Ψ_k Newsletter

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

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Contents

1 Editorial

In the **General News** section we have information on three different softwares, and among them the Vanderbilt pseudopotentials, the Carr-Parrinello Molecular Dynamics code, and the ABINIT project. In addition, there readers can also find the address of the web site presenting a video with interviews of Walter Kohn, after he received his Noble prize. In the section dedicated to **RTN2** ("Psi-k f-electrons") and **RTN3** ("Exciting") there are three position announcements related to these networks. More position announcements can be found in the usual **General Job Announcements** section. We have a number of various reports in the **TMR2** and **ESF** sections, some of them containing also abstracts of presented papers. In addition, abstracts can also be found in the usual **Abstracts** section. There are also two workshop announcements in the **General Workshop/Conference Announcements** section. The scientific highlight on **"Full-Potential Local-Orbital Minimum-Basis Scheme (FPLO)"** is by Klaus Koepernik, Helmut Eschrig, Ingo Opahle, Ulrike Nitzsche, Igor Chaplygin, and Manuel Richter (Dresden). Please check the table of contents for further details.

The *Networks* have a home page on World Wide Web (WWW). Its *Uniform Resource Locator* (URL) is:

http://psi-k.dl.ac.uk/

The above contains information on the Psi-k 2002 workshops and hands-on courses. In these pages you can also find information on how to apply for funding to make collaborative visits.

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

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

	function
psik-coord@daresbury.ac.uk	**messages to the coordinators, editor & newsletter**
psik-management@daresbury.ac.uk	**messages to the NMB of all Networks**
psik-network@daresbury.ac.uk	**messages to the whole Ψ_k community**

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2 General News

2.1 Video of Walter Kohn on the Web

at the Vega Science Trust http://www.vega.org.uk

The Vega Science Trust is a charity based at Sussex University that produces scientific videos. As part of our work we have been recording archive footage of eminent scientists, and our latest recordings are of Walter Kohn, 1998 Nobel prize winner in Chemistry for his work developing Density Functional Theory.

All of our videos are available to watch on the Web for free (they require the RealPlayer, which can also be downloaded for free, directions are on the Website). The address to view Walter is:

http://www.vega.org.uk/series/facetoface/kohn/

The site is a one hour extract from extensive recordings, and makes for fascinating viewing, as Walter talks to John Perdew about how he first developed DFT, how DFT works, and how he envisages its development and application in the future.

For those working in biology or nanotechnology we also have archive recordings on the site of Max Perutz, Fred Sanger, as well as nanotechnologists Harry Kroto, Sumio Iijima, Millie Dresselhaus, etc. There are also extensive lectures, workshops, masterclasses and debates on a variety of scientific subjects.

2.2 Vanderbilt Ultra-Soft Pseudopotential Web Site

David Vanderbilt

Department of Physics and Astronomy, Rutgers University

An open-source package consisting of codes for generating ultrasoft pseudopotentials, together with associated documentation and a pseudopotential library, is now posted at

http://www.physics.rutgers.edu/~dhv/uspp/

This is essentially the same package of source codes that has been distributed to colleagues on request for some years; previous versions had names like a7.3.2, where the numbers refer to a release sequence. These pseudopotentials are compatible with some open-source plane-wave packages (e.g., DACAPO, PWSCF) and also with several proprietary (e.g., CASTEP, CPMD) and private packages.

The library takes the form of a database of input parameter files that can be used to generate the pseudopontial datafiles, rather than the pseudopotential datafiles themselves. Thus, to obtain even one pseudopotential, you have to download and install the package and run the generation procedure for the atom of interest. However, the package has been designed so that this is easy to do.

Currently, the library includes pseudopotentials for approximately 20 atoms in the periodic table. However, contributions to the library from the user community are encouraged, and it is hoped that the database will expand rapidly to cover most of the periodic table.

2.3 CPMD Program Web Site

The updated version 3.5.2 of the CPMD program (Ab-initio Molecular Dynamics program, developed by J. Hutter, M. Parrinello et al., copyright IBM Corp and MPI Stuttgart) is now available at

http://www.cpmd.org.

New Features included in the update are:

-Interface to the new Vanderbilt pseudopotentials generation code
-Non Linear Core Correction (NLCC) with Vanderbilt pseudopotentials
-Vanderbilt pseudopotentials bugs fixed
-NEC optimization
-General Fixes

Any non-profit organization can obtain a free licence there.

Thank you to everyone who contributed to this new release.

Your cpmd.org team (http://www.cpmd.org)

2.4 The ABINIT Software Project

X. Gonze, for the ABINIT group (see below)

The first-principles computation of material properties, relying upon quantum mechanics and electromagnetism, has undergone tremendous progress in the past twenty years. In order to stay up-to-date, computer programs for first-principle study of materials must include more and more functionalities, that progressively become considered as “basic” functionalities. It is clear that improvements or generalisations of the DFT formalism, and/or its implementation, and/or its domain of application, will continue for the next decade or even longer. Group development is required, and even international collaboration. In this context, different modern software engineering techniques prove extremely useful.

The ABINIT software project was started in 1997, on this basis, as an open software project, without a “definite” goal, developed using several software engineering techniques to allow international collaboration of many different groups.

The main program of the ABINIT package performs density-functional calculations of material properties, using a plane-wave basis and pseudopotentials (PWPP). Beyond basic functionalities, often present in PWPP codes, ABINIT is able to deal with spin-polarized systems, spin-orbit coupling, Berry phase computation of polarisation, linear responses (automatic computation of phonon band structure, dielectric tensor, Born effective charges), excited states (TDDFT and GW approximation)... For a complete list of functionalities of the latest version, see

`http://www.abinit.org/ABINIT/Infos_v3.4/Features/features_v3.4.htm`

At present, this software is (1) open source software, or in other words, free software (available under the GNU General Public License, see http://www.gnu.org), (2) self-testing, (3) portable across platforms for serial and parallel execution, (4) self-documented. A self-learning procedure is provided to the user. A protocol for international group development has been set up, including an explicitly stated coding style. The Web site (http://www.abinit.org) provides the official versions, pseudopotentials, different utilities, benchmarking results, mailing lists (presently more than 350 addresses on the user mailing list) and bibliographical information.

Although more than 50 individuals, forming the ”ABINIT group”, have contributed to the project over the years, some people are clearly committed to it, including: X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic and M. Verstraete from the Université Catholique de Louvain, Belgium ; G. Zerah, F. Jollet, M. Torrent and A. Roy from the Commissariat à l’énergie atomique, Bruyères-le-Chatel, France; M. Mikami from Mitsubishi Chemical Corp., Yokohama, Japan; Ph. Ghosez, J.-Y. Raty, M. Veithen, from the Université de Liège, Belgium; D.C. Allan, from Corning Inc., USA; V. Olevano, L. Reining from l’Ecole Polytechnique, France.

3 News from RTNs 'Psi-k f-electron' (RTN2) and 'Exciting' (RTN3)

Ab-initio Computation of Electronic Properties of f-electron Materials (RTN2)

First-Principles Approach to the Calculation of Optical Properties of Solids (RTN3)

3.1 Position Announcements

3.1.1 Postdoctoral Positions in Aarhus

DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF AARHUS, DENMARK

Two Post-doctoral Positions

Condensed Matter Theory: Electronic Structure of f-electron Materials or Optical Properties of Solids

Applications are invited for two post-doctoral positions funded by the European Research Training Networks, **Psi-k f-electron**: '*Ab-initio Computation of Electronic Properties of f-electron Materials*' and **EXCITING**: '*First-Principles Approach to the Calculation of Optical Properties of Solids*', respectively.

The positions are available for a period of 1 year. Extension is possible. The start time is flexible, within the next year.

The applicant must comply with the RTN rules for network employment of young scientists: The applicant should hold a Ph.D. degree or equivalent in Physics or Chemistry, be aged 35 or younger, and should have some experience in computational Condensed Matter Theory. He/she must be of European Union nationality, or from one of the Associated Nations, or have resided in an EU country for the last five years or longer. Danish citizens are excluded, however.

The successful applicants shall participate in either of the above network projects. This implies applications of present computer codes to solid systems of high current interest as well as development of improved computer codes. The projects are collaborations in international teams and some travel activity between the research centers involved must be foreseen. More detailed information concerning the project can be obtained upon request.

The salary depends on seniority as agreed between the Danish Ministry of Finance and the Confederation of Professional Unions.

Applications should include a curriculum vitae, giving evidence on which the evaluation of the applicant's scientific qualifications can be based, a complete list of publications with an indication of those which the applicant selects as the most relevant for the application. The applicant must, upon request, submit further material required by the selection committee in its evaluation.

For further information, contact:

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Email: svane@phys.au.dk or nec@phys.au.dk

Information about the Institute can also be found on http://www.phys.au.dk.

3.1.2 Postdoctoral Position in Dresden

Postdoc Position in Theoretical Solid State Physics

IFW Dresden, Germany

We would like to announce an open postdoc position in the framework of the European Research Training Network

"Ab-initio Computation of Electronic Properties of f-Electron Materials."

The applicant should be a non-German citizen of the European Community or an associated state and should not have worked in Germany for more than 12 months during the last two years. (The precise regulations are found at `http://www.cordis.lu/improving/networks/faq.htm#q5` .)

The project, to be carried out at IFW Dresden (http://www.ifw-dresden.de) in cooperation with 7 other network partners in Europe and USA, includes

1. density functional studies of surface magnetism on lanthanide elements and compounds, using the recently developed FPLO code (http://www.ifw-dresden.de/FPLO/);
2. code development with respect to surface-specific properties and tasks.

Close contact with related experimental work at IFW Dresden, University of Technology Dresden (http://www.tu-dresden.de), and the Max-Planck Institute for the Chemical Physics of Solids Dresden (http://www.cpfs.mpg.de) is envisaged, as well as collaboration with several Dresden groups active in solid state theory.

The applicant should preferably have a safe background in solid state physics, good knowledge of density functional theory, and experience in the understanding and development of extended code for numerical purposes (FORTRAN 90 and/or C).

We offer a one-year position, extendable up to 3 years, at the level BAT IIa-O (annual net income about kEUR 20, depending on age and family status), as well as relocation and regular travel costs to the home scientific community of kEUR 7 in total.

The Department of Theoretical Solid State Physics at IFW Dresden consists of eleven PhDs in solid state theory, three PhD students, and several guest scientists, see http://www.ifw-dresden.de/agtheo/eagtheo1.htm. The group has up-to-date computer facilities, daily coffee meetings, and a lively exchange with a number of other groups inside and outside of Dresden (theoretical and experimental, physics and chemistry). The city of Dresden is situated mid-way between Berlin and Prague, in the valley of river Elbe. With a population of about 500,000, it is known for a rich cultural live and for its baroque silhouette.

Interested candidates should send their application together with a curriculum vitae, a list of publications or current research activities, and other relevant material to:

Dr. Manuel Richter
Dept. of Theoretical Solid State Physics
IFW Dresden e.V.
P.O. Box 270016
D-01171 Dresden, Germany
email m.richter@ifw-dresden.de

4 News from the TMR2 Network

'Electronic Structure calculations of materials properties and processes for industry and basic science'

4.1 Reports on Participation in Conferences/Workshops

4.1.1 Report on attending SCES'02 Conference

International Conference on Strongly Correlated Electron Systems (SCES)

10-13 July, 2002, Krakow, Poland

The conference took place at the 640 years old Jagiellonian University in the beautiful city of Krakow, Poland. It opened with an evening reception on July 9, 2002, but the scientific programme started on July 10, 2002. The conference was attended by about 350 participants from all over the world, with about one third from Japan! It was run in single morning sessions and two parallel afternoon sessions, with the exception of the last day when only the plenary and invited talks were presented in a single session run throughout the day. In total there were 6 plenary-, 23 invited-, and 61 contributed talks. The remaining papers were presented during two evening poster sessions. The morning sessions started with a plenary talk of 50 minutes, followed by 4 invited talks of 30 minutes each. The afternoon sessions started with an invited talk, followed by 10-11 contributed talks of 15 minutes each. On the last day of the conference there were 3 plenary talks, and 4 invited talkes, followed by two conference summaries of 30 minutes, delivered by P. Fulde (Dresden) for the theory part, and J. Franse (Amsterdam), (giving introduction and summarizing the experimental work concerned with magnetic order), J. Flouquet (Grenoble) (summarizing heavy fermion and superconductivity papers), and G. Lander (Karlsruhe) (presenting a summary for the NMR and spectroscopies) for the experimental part, which was a nice way of wrapping up the SCES'02 conference.

The scope of the conference was very broad, comprising such subject topics as exotic superconductors (ESC), heavy fermions and other intermetallic $f-$electron compounds (HF), Kondo impurity and lattice systems (KON), magnetism (MAG), Mott-Hubbard systems (MOT), non-Fermi liquid behaviour (NFL), novel materials (NM), systems with orbital degrees of freedom (manganites) (OO), correlated quantum dots and other mesoscopic systems, Hall liquids (QD), quantum phase transitions and quantum liquids (QPT), and finally superconductivity and its coexistence with magnetism (SCF). Five of the above subject topics were represented in the plenary talks. First plenary talk was delivered by F. Steglich (Dresden) on "UBe_{13}: Prototype of a non-Fermi liquid superconductor" (NFL). It addressed the issue of NFL and its coexistence with HF superconductivity before discussing in detail the experimental situation of UB_{13}, its doping with Th, and the effects it had on the superconductivity. The other plenary talks were by J. Flouquet (Grenoble) on "Ferromagnetic superconductors" (SCF), T. Moriya (Tokyo) on "Spin fluctuations and superconductivity around the magnetic instability" (ESC), G.A. Sawatzky (Vancouver) on "Stumbling trajectory in the Mott-Hubbard-Anderson electron correlation problem" (MOT), Y. Tokura (Tokyo) on "Control of the Mott transition in transition-metal oxides" (OO), and C.M. Varma (Murray Hill) on "Issues in quantum critical phenomena in heavy fermions and in the cuprates" (NFL). This latter talk gave, among others, a very comprevensive, pedagogical introduction to quantum critical phenomena. In the Flouquet's talk, apart from such systems as UGe_2, URhGe (possibly close to quantum critical point), $ZrZn_2$, he also mentioned possible existence of superconductivity in the hcp (ϵ phase) Fe, and $\alpha-$U. The theme of ferromagnetic superconductors was continued in a contributed talk by D. Aoki (Grenoble) et al. on "Superconductivity of the itinerant ferromagnet URhGe", and in a number of posters. Moriya reviewed the spin fluctuation theory and its relevance to superconductivity around magnetic instability and quantum critical point, with the emphasis on high-T_c cuprates. It was concluded that superconductivity of the latter and their high-T_c's could be consistently explained in terms of spin fluctuations, as could also be the differences between the electron- and hole-doped cuprates. A Hubbard model with an intermediate coupling interaction appeared to be a good and consistent model for cuprates with spin fluctuations, while t-J model might be insufficient for doped cuprates. G.A. Sawatzky gave a historical review of the Mott-Hubbard-Anderson electron correlation problem, finishing with new results showing that even CaO, a large gap nonmagnetic material, can, upon introducing a small concentration of Ca vacancies, exhibit extraordinary properties like half-metallic ferromagnetism. Finally, Y. Tokura discussed band filling control of Mott transition in oxide perovskites, Mott-insulator transitions caused by orbital ordering, orbital ordering vs. orbital liquids, order-disorder transitions. Manganites featured also in a number of posters and the contributed talks by: J.M. De Teresa (Zaragoza) et al. on "Dynamic cluster effects in manganites probed by small-angle neutron diffraction" (OO), B. Dabrowski (DeKalb) et al. on "Correlation of magnetic transition temperatures to structural and charge disorder for perovskite manganites" (OO), and R. Frésard (Caen) et al. on "Large negative thermopower in electron-doped manganites" (OO).

It seems that majority of papers presented at the conference were concerned with experimental studies. A vast amount of work was on the heavy fermion materials, mostly U- and Ce-based compounds, but Yb-compounds, cuprates and other transition metal oxides (e.g. manganites) were also studied. Among the heavy fermion materials there were those long known and studied like UB_{13} and UPt_3, but there were also new ones like skutterdudites, RT_4X_{12} (R-rare earth, T=Fe, Ru, Os, X=P, As), especially Pr-based compound ($PrOs_4Sb_{12}$), which J. Flouquet in his summary called a new gold rush of this conference. The quantum critical phenomena, and the occurance of the superconducting phase around the quantum critical point, coexistence of magnetism and superconductivity, the recurring theme of heavy fermion physics, were well represented in many papers, be it plenary, invited or contributed. The studies were performed mostly on the bulk materials, but there were a few on mesoscopic systems, mostly from Polish participants. The experiments were performed at high magnetic fields or pressures. Techniques used included spectroscopies, like photoemission, Raman, XAS, XMCD, etc., Mössbauer technique, ESR, NMR, NQR, de Haas van Alphen technique, neutron scattering-, specific heat-, magnetization-, resistivity measurements, and others. In general, one could observe many large, international collaborations in many presented papers. Among the talks based on the experimental studies, the invited talk on "Hidden Order in URu_2Si_2" (QPT) by J.A. Mydosh (Leiden) reviewed the latest results on the 'mysterious' phase transition in this system which remains unexplained, and hence the name "hidden order". This compound was also reported in a contributed talk by M. Jaime (Los Alamos) on "Specific heat and magneto-caloric effect of URu_2Si_2 across the 35-40 T metamagnetic transition" (HF), as well as in posters. Y. Ōnuki (Osaka) presented an invited talk on "de Hass van Alphen experiments in the quantum critical region of cerium and uranium compounds" (QPT) and discussed changes of the electronic states under pressure when approaching the critical value of P_c, at the quantum critical point region. H. von Löhneysen (Karlsruhe) in his invited talk on "Investigation of the quantum phase transition in $CeCu_{6-x}Au_x$" (QPT) discussed tuning of magnetic instability by alloying or applying external pressure, and explaining the observed non-Fermi liquid behaviour by the quasi two-dimensional (2D) critical fluctuations, while three-dimensional (3D) fluctuations are associated with field-tuned quantum critical point. N. Bernhoeft (Grenoble) presented an invited talk on "Introducing the concept of a dynamical phase in magnetic order: possible implications for URu_2Si_2" (MAG), trying to explain asymmetric shift in the position of the magnetic scattering wave vector with respect to the lattice, observed in the diffraction experiments in the vicinity of antiferromagnetic phase transitions. The invited talk by V. Sechovský (Prague) reviewed "Pressure induced phenomena in U intermetallics" (MAG). R. Troć (Wroclaw) discussed "Magnetic fluctuations in the ordered state of the ferromagnetic superconductor UGe_2" (SCF). The latter compound was also discussed in a contributed talks by T. Terashima (Tsukuba) et al., entitled "Fermi surface studies of the ferromagnetic superconductor UGe_2 under high pressure" and R. Settai (Osaka) et al. on "de Haas van Alphen experiments under pressure in UGe_2" (QPT), and in posters. M.B. Maple (San Diego) in his invited talk was concerned with "Superconductivity and heavy fermion behaviour in $PrOs_4Sb_{12}$" (HF), possibly identifying the first Pr-based heavy fermion superconductor. Skutterrudites were also a subject of the invited review talk by E. Bauer (Vienna), entitled "Filled skutterudites: ground state properties and thermoelectric features" (NM), and contributed talks by K. Iwasa (Tokyo) et al. on "Antiferro-quadrupolar ordering of $4f-$electron state in the filled skutterudite $PrFe_4P_{12}$" (HF), and H. Sato (Tokyo) et al. on "Magnetic field effect on the transport properties of the anomalous heavy fermion $PrFe_4P_{12}$" (HF). M. Nicklas (Los Alamos) had an invited talk on "Relationship of magnetism and superconductivity in heavy-fermion systems: Pressure studies on $CeMIn_5$ and $CeMIn_8$ (M=Co, Rh, Ir)" (HF), pointing out remarkably high superconducting temperatures in these compounds compared to other heavy fermion superconductors. These systems featured also in the contributed talk by G.-q. Zheng (Osaka) et al. on "Unconventional superconductivity and quasi two-dimensional magnetic fluctuations in Ce(Ir, Rh)In_5", reporting extensive NQR/NMR studies. The invited talk by P. Gegenwart (Dresden) was on "Divergence of heavy quasiparticles at the quantum critical point in $YbRh_2Si_2$" (NFL), this system showing pronounced non-Fermi liquid effects in thermodynamic, magnetic, and transport properties. The latter system was also featured in a contributed talk by M.M. Abd-Elmeguid (Köln) et al. on "Pressure induced long range magnetic order in the non-Fermi liquid system $YbRh_2Si_2$" (NFL). The long known and studied band ferromagnet $ZrZn_2$ was a subject of the invited talk by C. Pfleiderer (Karlsruhe) on "Zero temperature magnetic to nonmagnetic phase transitions in d-electron ferromagnets" (QPT) that reported superconductivity in the mK range in ultra-pure samples of this material. D. van der Marel (Groningen) in his invited talk addressed "Low frequency conductivity of (non)-Fermi liquids" (NFL), featuring $\alpha-$ and $\gamma-$Ce, MnSi, and 2D cuprate superconductors. At this point it is also worthwhile to mention a contributed talk by N. Jaouen (Grenoble) et al. on "Soft X-ray resonant magnetic reflectivity at Fe $2p$ and Ce $3d$ core level in Ce(α)/Fe and Ce(γ)H_2/Fe" (MAG), probing the $\alpha-$phase and $5d$ magnetic profile in Ce/Fe multilayers and $4f$ magnetism in CeH_2/Fe multilayers. The invited talk by A. Fujimori (Tokyo) on "Novel electronic structure in the vicinity of metal-insulator transition in the high T_c cuprates" (MOT) discussed, on the basis of photoemission results, how the electronic structure evolves from the Mott insulator to metal (superconductor) in the layered cuprates, from the lightly-doped to underdoped regions. P. Wachter's (Zürich) invited talk was on "A superfluid in condensed excitonic state in intermediate valent $TmSe_{0.45}Te_{0.55}$" (HF), based on the the thermal conductivity and thermal diffusivity measurements. Finally, A. Loidl (Augsburg) discussed the issue of "Heavy-fermion formation in transition metal oxides", (MOT) and comparing experimental data with recent theoretical models presented evidence that the d-derived heavy-fermion formation occurs in frustrated magnets, in systems close to a metal-insulator transitions, as well as in systems close to quantum critical point.

The theoretical work was mostly based on models like the Hubbard and Anderson models, t-J model, the Falicov-Kimball model, tight-binding models, FLEX, etc. Also the crystal electric field (CEF) approach was used in a number of contributions, mainly by the group of R. Radwanski (Krakow), applied to $4f-$electron intermetallics, etc. The orbitally degenerate Hubbard model was used by T. Hotta and K. Ueda (Tokai, Kashiwa) to study triplet superconductivity of $f-$electron systems in their contributed talk on "Effect of orbital degeneracy on triplet superconductivity in $f-$electron systems" (SCF). In fact, the Hubbard model was used in many papers. The Falicov-Kimball model, in the dynamical mean field theory (DMFT) implementation, featured in the invited talks by V. Zlatić (Zagreb) on "Theory of Yb- and Eu-based intermetallics with unstable $4f-$shells" (HF) and J.K. Freericks (Washington DC) on "Inelastic light scattering and the correlated metal insulator transition" (MOT), the latter foccussing on the Raman response. In the application by Zlaticć this simple model failed to capture the valence-fluctuating features of the studied compounds. The Falicov-Kimball model was also used as an example in a contributed talk by A.M. Shvaika (Lviv) on "Dynamical mean field theory of correlated hopping: rigorous local approach" (MOT), as well as in posters. P. Prelovšek (Ljubljana) in his invited talk on "Spectral functions and pseudogap in models of strongly correlated electrons" (NFL) used t-J model, as relevant to cuprates, to calculate spectral functions, and discussed them in relation to a pseudogap and its coexistence with the Fermi liquid behaviour. P. Coleman (Rutgers) gave an invited talk on "Probing the break-up of the heavy electron at the quantum critical point" (QPT), discussing how the Fermi liquid evolves into the quantum critical point and outlining constraints on a future theory of this phenomenon. In the invited talk on "The Kondo-lattice model and the Kondo-spin glass competition in heavy fermion systems" (KON) B. Coqblin (Orsay) reviewed the main features of the Kondo lattice model in the mean field treatment of the Hamiltonian, discussing also the nature of the transition at the quantum critical point, and presenting comparison with experiments for heavy fermion systems. C. Lacroix (Grenoble) ("Geometrical frustration and heavy fermions" (HF)) used a model with geometrical frustrations, that included both itinerant and localized electrons, to describe heavy fermion behaviour not related to the Kondo effect, of relevance to such systems as LiV_2O_4. Also, G. Zwicknagl (Braunschweig) presented a contributed paper on "The dual nature of $5f$ states and heavy quasiparticles in UPt_3" (HF) in which she used a combined microscopic approach to treat one of the $5f$ electrons as itinerant, while others were considered to be localized. She concluded that the enhancement of the quasiparticle effective masses over the band mass results from the local Coulomb interaction of the itinerant $f-$states with their localized counterparts, while the Fermi surface is determined entirely by the itinerant $5f$ states.

The papers using the ab-initio approach of the density functional theory were in the minority. There was one invited talk, using the LDA+DMFT approach, presented by D. Vollhardt (Augsburg) on "Realistic modeling of materials with strong electronic correlations" (MOT). He presented recent results for photoemission and inverse photoemission spectra of transition metal oxides such as $La_{1-x}Sr_xTiO_3$ and V_2O_3, and for the spin state and orbital occupation of paramagnetic V_2O_3 across the Mott-Hubbard transition. The contributed talk by M.D. Johannes and W.E. Pickett (Davis) on "Magnetic ordering in quadruple perovskite $CaCu_3Ti_4O_{12}$" (MAG) tried to understand the antiferromagnetic order in this compound using a tight-binding fit (with 7 neighbours) to an accurate first-principles band structure calculations, revealing the superexchange coupling between 5th Cu-Cu neighbours. In the contributed talk by H. Harima (Osaka), K. Takegahara (Hirosaki), K. Ueda (Kashiwa), and S.H. Curnoe (Kashiwa and Newfoundland) on "Origin of the metal-insulator transition in $PrRu_4P_{12}$" (HF) the FP-LAPW-LDA+U method was used to discover that the metal-insulator transition in this skutterudite compound was caused by a perfect 3D nesting of the Fermi surface. The ab-initio band structure calculations featured also in a number of poster presentations. Among them was the study on "High temperature expansions for the J_1-J_2 Heisenberg models: application to ab-initio calculated models for Li_2VOSiO_4 and Li_2VOGeO_4" (MAG) by H. Rosner (Davis), R.R.P. Singh (Davis), W.H. Zheng (Sydney), J. Oitmaa (Sydney), S.-L. Drechsler (Dresden), W.E. Pickett (Davis), using the exchange couplings calculated within LDA and showed that the measured Néel temperature was consistent with the LDA-derived J-perpendicular. H. Yamagami (Kyoto) presented relativistic spin-polarized calculation of the Fermi surface for $UPtGa_5$ compound using the LAPW method, in the poster on "Fermi surface of antiferromagnet $UPtGa_5$ in relativistic spin-polarized band theory" (HF). He concluded that this compound should be $5f$ itinerant antiferromagnet. J. Deniszczyk and W. Borgiel (Katowice) studied "The heavy-fermion properties of the $Fe_{3-x}V_xAl$ alloys" (HF) with the FP-LAPW band structure method. A. Yaresko (Dresden) presented a poster on "The LDA+U band structure of UPd_3" (HF). Our poster on "SIC-LSD Study of Correlated Transition Metal Oxides" (MAG) by Z. Szotek (Daresbury), W.M. Temmerman (Daresbury), A. Svane (Aarhus), and H. Winter (Karlsruhe) was concerned with the self-interaction corrected (SIC)-LSD first-principles study of valencies and magnetic and/or charge orders in such systems as half-metallic double perovskites, magnetite, and YBCO. It is probably worthwhile to mention that, the TB-LMTO band structure method was used in a number of papers, oral and posters, for performing calculations to support interpretation of experimental data.

In summary, I found the conference very useful, although rather tightly packed with talks and poster sessions which, despite a very hot weather, were well attended over all four days. Of course, it is nearly impossible to at least mention all interesting papers presented at the conference, and one has to stop at some point. However, besides the scientific part, the conference dinner deserves to be mentioned. It took place in a typical country restaurant in one of the villages outside Krakow, and was a definite highlight of the conference, with traditional food and folklore dancing and singing, a well deserved break after heavy sessions of the conference. I appreciated very much the opportunity to participate in this interesting, and well organized, conference and would like to acknowledge a financial support from the EU through the TMR2 Network.

Z. (Dzidka) Szotek

July, 2002

5 News from the ESF Programme

"Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces"

5.1 Reports on Workshops/Conferences

5.1.1 Report on the Mini-Colloquium "Mineralogy and Geophysics"

CMD19/CMMP2002 SESSION "MINERALOGY AND GEOPHYSICS"
Brighton 7-11 April 2002

Sponsored by European Science Foundation "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" (Psi-k)

Organized by
Lubomir Benco, Vienna University, Austria
Björn Winkler, Frankfurt University, Germany

The aim of the mini-colloquium was to gather geophysicists and electronic-structure scienticsts thus supporting the interdisciplinary scientific exchange and the establishment of a common language for mineralogy oriented researchers.
The colloquium consisted of 5 talks, two ivited (30') and three contributing presentations (20'). The contributions demonstrate that two main directions have been emerging in computational mineralogy and geophysics. Application of ab-initio calculations to larger and more complicated systems (contribution 1 and 3) and development of novel Monte Carlo approaches to characterize specific properties of materials (contribution 2, 4 and 5).

Program
CMD19CMMP2002: Thursday Morning, 11th April 2002

8:30 **Session Opening (L. Benco)**
8.32 **D Alfe (University College London, UK)**
The composition of the Earth's core from first principles calculations
9:00 **MT Dove (University of Cambridge, UK)**
Low-energy excitations of crystalline and amorphous silicates
9:30 **C Ganarelli (University College London, UK)**
Ab initio thermodynamics of iron at Earth's core conditions by the "particle-in-cell" approximation
9:50 **IT Todorov (University of Bristol, UK)**
New approaches to the simulation of solid solutions at high pressure

10:10 MYu Lavrentiev (University of Bristol, UK)
Application of novel Monte Carlo methods to disordered minerals and solid solutions

10:30 End of Session

Abstracts

The Composition of the Earth's Core from First Principles Calculations

D Alfe, MJ Gillan, GD Price, *University College London, UK*

The composition of the Earth's core is one of the main problems in the geological sciences. We know that the core is mainly formed by iron, but it must also contain some light elements because its density is lower than the density of pure iron. We have used *ab initio* methods to put some constraints on the possible composition of the core. The constraints stem on the fact that at the boundary between the solid and the liquid the chemical potentials of all the elements must be equal in the two phases. This condition fixes the partitioning between liquid and solid of possible candidate light element(s). A comparison with the density of the liquid and the solid core, known accurately from seismological data, determines the constraints. We show that no binary mixture Fe/S, Fe/Si or Fe/O is possible, and we propose a possible composition of the Earth's core containing $\approx$ 8% S/Si in the solid, and $\approx$ 10% S/Si plus $\approx$ 8% O in the liquid. The temperature of the inner core boundary (ICB) has been estimated in the past by referring to the melting temperarure of pure iron at ICB pressure. This partitioning of light elements between solid and liquid shifts the melting temperature of the mixture by about -700 K with respect to the melting temperature of pure iron. The methods described here are completely general, and should find wide applicability in a number of geological problems related with coexistence of phases.

Low-Energy Excitations of Crystalline and Amorphous Silicates

Martin Dove, *University of Cambridge, UK*

The structures of silicates can be described as consisting of a network of corner-linked tetrahedral SiO4 and AlO4 structural units. These units are very stiff, and any low-energy deformation will need to involve flexing of the network without distortions of the structural units. A simple engineering analysis suggests that these networks are on the boundary between being rigid and flexible, and in fact they are slightly floppy. This floppiness allows some phonons to act as soft modes for displacive phase transitions. It has recently become apparent that silicate glasses have the same flexibility as crystalline silicates, and in fact there are some aspects of the low-energy dynamics of silicate glasses that are remarkably similar to the dynamics of their crystalline counterparts. A picture has emerged of the dynamic properties of these materials based on a combination of lattice dynamics, molecular dynamics and reverse Monte Carlo modelling techniques.

Ab initio Thermodynamics of Iron at Earth's Core Conditions by the 'Particle in a Cell' Approximation

C Ganarelli, D Alfe, MJ Gillan, *University College London, UK*

The particle-in-cell approximation has the potential to massively simplify ab initio calculations of the thermodynamic properties of materials. The present work attempts to evaluate the usefulness of the particle-in-cell approach, by comparison with the more rigorous technique of thermodynamic integration.

Applications of Novel Monte Carlo Methods to Disordered Minerals and Solid Solutions

NL Allan(1), Z Du(1), MYu Lavrentiev(1), JA Purton(2), IT Todorov(1)
(1)School of Chemistry, University of Bristol, (2)CLRC, Daresbury Laboratory

A key problem in the modelling of geologically important materials is a proper description of disorder, and its variation with temperature and pressure. Recently we have implemented a number of novel Monte Carlo approaches and we present here a summary of our recent results [1].

Our main tool is exchange Monte Carlo, which allows for random exchanges of cations in addition to random ion moves and changes in the size of the simulation box. We have carried out comprehensive studies of the oxide solid solutions MgO/MnO and MgO/CaO. In MgO/CaO, for example, the large difference in ionic radius between Mg2+ and Ca2+ results in a low rate of successful exchanges and so a configuration-bias approach has been implemented. We have thus calculated the phase diagram for both solid and liquid phases. For normal and inverse spinels, where heterovalent exchange takes place (non-convergent ordering), we have investigated the temperature and pressure dependence of the order parameter. Simulations of garnet solid solutions have also been carried out, demonstrating the effects of ordering in 50/50 pyrope-grossular mixtures.

We also present results for the incorporation mechanisms of noble gases in silicate minerals and melts. Here we have used grand-canonical Monte Carlo to obtain noble gas-silicate potentials.

[1] N.L. Allan, J.D. Blundy, J.A. Purton, M.Yu. Lavrentiev, B.J. Wood. In: C.A. Geiger (ed.): Solid solutions in silicate and oxide systems (EMU Notes in Mineralogy, 3), p. 251 (2001).

New Approaches to the Simulation of Solid Solutions at High Pressure

IT Todorov, NL Allan, *University of Bristol, UK*

We show how a configurational lattice dynamics technique [1,2], in which the free energy of a number of configurations is determined directly by means of fully-dynamic structural minimizations, can be used to calculate thermodynamic properties of solid solutions and phase diagrams at high temperatures and high pressures.

The accurate calculation of the free energy of periodic solids and slabs via lattice statics and quasiharmonic lattice dynamics [1,2] is quick and computationally efficient and does not resort to lengthly thermodynamic integration. It is also an attractive strategy for temperatures below the Debye temperature where classical Monte Carlo fails due to neglect of quantum effects. Our new code calculates the full set of free-energy first derivatives analytically and so full minimization of the quasiharmonic free energy with respect to all internal and external variables is possible for large unit cells. The program currently uses conventional two and three-body rigid-ion and shell-model potentials.

Our configurational lattice dynamics approach [1,2] to solid solutions thus involves thermodynamic averaging over the results of a limited set of free-energy minimizations of different arrangements of the cations within the cell. In our approach no assumptions are made as to the nature of the solution and both configurational and vibrational entropy contributions are determined directly. We show how crucial are local relaxation effects for the formation of ionic solid solutions and how vibrational effects influence thermodynamic properties. We also show how the extension of our approach to interfaces can be employed for calculation thermodynamic properties at surfaces of solid solutions.

The method is illustrated using the ceramic system MnO/MgO, for which our results strongly support the recent experiments of Wood et al. at Bristol, who, unlike previous workers, suggest the formation of a complete solid solution at temperatures only above 1000K. Calculated thermodynamic properties are compared with those obtained using a Monte Carlo technique [1-3], and results are presented for zero pressure and 50 GPa. Vibritaional contributions to different thermodynamic properties are explicitly calculated, as a difference of lattice dynamics and lattice statics data, and results are presented for zero pressure and 50 GPa. Also shown are results for segregation energies of MnO/MgO and NiO/MgO at (001) MgO surface. In the former case, strong surface segregation of Mn2+ is predicted.

[1] N. L. Allan , G. D. Barrera, M. Yu. Lavrentiev, I. T. Todorov and J. A. Purton, J. Mater. Chem., 11 (2001) 63-68.

[2] N. L. Allan, G. D. Barrera, R. M. Fracchia , M. Yu. Lavrentiev, M. B. Taylor, I. T. Todorov and J. A. Purton, Phys. Rev.B, 63 (2001) 094203

[3] M. Yu. Lavrentiev, N. L. Allan , G. D. Barrera, J. A. Purton, J. Phys. Chem. B, 105 (2001) 3594-3599

5.1.2 Report on the Mini-Colloquium “Magnetoelectronics”

EPS/CMMP Conference 2002
Brighton 7-11 April 2002

Sponsored by
European Science Foundation “Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces” (Psi-k)

Organized by
A. Fert (Orsay), L. Molenkamp (Wuerzburg), P.H. Dederichs (Juelich)

The Mini-Colloquium consisted of four invited talks, the abstract of which are attached below. In the first invited paper (“Half-metallic ferromagnetic oxides for magnetoelectronics: Material’s issues”) J. Fontcuberta reported, that the tunnel magnetoresistance of tunnel junctions based on half-metallic oxides greatly increased due to improvement of the interfaces. In his paper “Materials-specific theory for spin electronics” P.J. Kelly discussed the description of spindependent transport in layered systems based on the Landauer-Buettiker formalism and using the tight-binding LMTO method, with applications to GMR and TMR, Andreev reflection and spin injection. Peter Levy highlighted in his paper “Spin-polarized current-driven switching of magnetic layers” the present understanding of the magnetization switching by a spin polarized current, stressing the differences between the longitudinal and transversal spin accumulation. D. Ferrand (“Ferromagnetic semiconductors”) reported recent progress in the young field of dilute magnetic semiconductors, by considering Mn-doped III-V semiconductors (GaAs, InAs) as well as II-VI ones (CdTe quantum wells and ZnTe epilayers).

The mini-colloquium was rounded of by a quite good poster session of 19 experimental and theoretical contributions. Due to the many other mini-colloquia, in total the EPS conference was interesting and successful, although the organization was not perfect.

Peter H. Dederichs

Half-metallic ferromagnetic oxides for magnetoelectronics: Material’s issues

J. Fontcuberta, M. Bibes, S. Calncia, Ll. Balcells, J. Santiso, B. Martnez, E. Jedryka[⋆], M. Wojcik[⋆], M.J. Casanove[†]
CSIC, Spain
[⋆]*Polish Academy of Sciences, Poland*
[†]*CNRS, France*

Half-metallic ferromagnetic oxides such as the celebrated manganites, have created great expectations for its potential use as ferromagnetic electrodes in the emerging field of magnetoelectronics. However, the performance of F/I/F tunnel devices based on manganites is far from ideal. The tunnel magnetoresistance decays rapidly when rising the temperature and becomes negligible at room-temperature or well below the corresponding Curie temperature. In this presentation we shall discuss some material's aspects of the manganite thin films and heterostructures. Particular emphasis will be devoted to issues such as the electronic/magnetic homogenity of films at or close to interfaces with the insulating (I) barriers or substrates. We will overview strategies and efforts to overcome these difficulties. In any event, materials having still higher Curie temperatures are needed. Recent progress on thin film growth of alternative half-metallic ferromagnetic oxides such as the double perovskites (Sr_2FeMoO_6) or magnetite (Fe_3O_4) will be reviewed.

Materials-specific theory for spin electronics

P.J. Kelly
University of Twente, The Netherlands

In the Landauer-Buettiker (LB) formulation of transport theory, the conductance of a system sandwiched between two leads is expressed in terms of the transmission matrix t. The (i, j)-th element of this matrix describes the probability amplitude for a propagating state i in the left hand lead to be transmitted into a propagating state j in the right hand lead. In this presentation, I discuss the application of the LB formalism to the calculation of spin-dependent electrical transport in layered magnetic materials. The transmission matrix is calculated from first-principles within the local density approximation of density functional theory. The efficient implementation using tight-binding linear-muffin-tin orbitals allows us to model interface and bulk disorder using large lateral supercells whereby specular and diffuse scattering are treated on an equal footing. I discuss applications to a number of topics of current interest: Giant and Junction Magnetoresistance; Andreev reflection at an interface between a ferromagnet and a superconductor; current induced magnetization reversal; spin injection from a ferromagnet into a semiconductor.

Spin-polarized current-driven switching of magnetic layers

P.M. Levy, A. Shpiro, S. Zhang*, A. Fert†
New York University
**University of Missouri*
†*Universite de Paris-Sud*

The concept of switching the orientation of a magnetic layer of a multilayered structure by the current perpendicular to the layers was introduced by Slonczewski and Berger, and has been followed up by Waintal et al. The central idea is that a spin polarized current exerts a torque on the magnetic moment of a layer if the spin polarization of the current is not oriented along the magnetization axis of the layer; this is a reflection of the exchange interaction between conduction electron spins and the local moments. An alternate mechanism of current induced switching was put forth by Heide in which the current across a magnetically inhomogeneous multilayer produces a longitudinal spin accumulation which establishes an energy preference for a parallel or antiparallel alignment of the moments of the magnetic layers; this magnetic "coupling" was posited to produce switching. Recent experiments have reliably demonstrated that the magnetization of a magnetic layered structure is indeed switched back and forth by an applied current. However, it is unclear whether the magnetization switching is triggered by the current induced magnetic coupling or by the "spin transfer" mechanism or both.

We have developed a model that relates the current-induced torque to the transverse spin accumulation that arises from driving a current across a magnetically inhomogeneous structure, i.e., the portion of the accumulation perpendicular to the local magnetization axes. We find that this torque has two components: the first one is similar to the torque predicted by Slonczewski and Berger; the second is mathematically similar to the torque in Heide's model, although its origin is different. The salient difference between our treatment and previous treatments of spin accumulation, lies in the inclusion of the exchange interaction between the spin accumulation and the magnetic background. Our two terms are derived simultaneously in the same formalism and both depend on the same set of parameters used for understanding the giant magnetoresistance when the current is perpendicular to the plane of the layers (CPP). Furthermore, we have introduced a new length scale for the transverse spin accumulation and clarified the ferromagnetic layer thickness dependence of the switching dynamics.

We present the two components of the torque, and the longitudinal and transverse spin accumulations for two ferromagnetic layers with a non-magnetic spacer between them. These quantities are sensitive to: the relative thicknesses of the magnetic layers, and the amount of interface scattering (reflection, transmission and diffuse) relative to that in the bulk magnetic layers and its spin dependence. The scattering at interfaces produces discontinuities in the transverse as well as the longitudinal spin accumulation, and thereby produces a torque an the background magnetization as well as contributing to the CPP resistivity and magnetoresistance. Among the noteworthy results we present are: the thickness-dependence of the two components of the torque to see in which region one dominates over the other, and their angular dependence; this is quite different from that used by those who have made micromagnetic simulations in which a simple expression might be misleading in determining the switching field. In the simple case where each magnetic layer is described by a magnetic moment of fixed magnitude we find the time dependence of the switching of a magnetic layer due to the torques created by the spin-polarized currents in magnetic multilayered structures.

Ferromagnetic semiconductors

D. Ferrand, H. Boukari, M. Bertolini, H. Mariette, S. Tatarenko, A. Wasiela, E. Kulakov, G. Firshman, M. Sawicki, T. Dietl*, P. Kossacki†, J. Gaj†, B. Barbara‡
Laboratoire de Spectrometrie Physique, BP 87, France
**Polish Academy of Sciences Al Lotnikow, Poland*
†*University of Warsawa, Poland* ‡*CNRS, France*

Diluted magnetic semiconductors (D.M.S.), where ferromagnetic interactions can be controlled externally by electronic gates, appear actually particularly attractive to manipulate and control the spin of the carriers in semiconducting devices [1]. Up to now, the Curie temperatures observed in well characterized III-V and II-VI D.M.S. remain far below room temperature (up to 110K in GaMnAs). But, the recent reports of much higher Curie temperatures in new D.M.S. alloys (GaMnN, ZnCoO [2]), support by theoretical predictions [3], have strongly stimulated the efforts on the growth of magnetic semiconductors. In this presentation, we will present first a review of the magnetic and electronic properties III-V ($Ga_{1-x}Mn_xAs$, $In_{1-x}Mn_xAs$ epilayers) and II-VI D.M.S ($Cd_{1-x}Mn_xTe$ quantum wells and $Zn_{1-x}Mn_xTe$ epilayers). In both materials, Mn atoms introduce localized spins, which are ferromagnetically coupled by RKKY exchange interactions, mediated by the holes situated in the valence band. A mean field treatment leads to a magnetic phase diagram versus the hole density and its dimensionality and Mn content, in good agreement the experimental studies.[2] For a given hole density and Mn content, the Curie temperature depends strongly on the valence band structure and the mean field models, which are currently confronted to ab-initio calculations, predict the possibility to achieve room temperature ferromagnetism with high gap D.M.S alloys (ZnMnO, GaMnN). We will finally present our first results on the growth and on the characterization of GaMnN epilayers.

[1] H. Boukari et al Cond-mat/0111511 27/11/2001 and H. Ohno et al, Nature **408**, 944 (2000)

[2] S. Sonoda et al Cond-mat/0108159 and K. Ueda et al, PASPS Sendai 2000

[3] T. Dietl et al, Science **287**, 1019 (2000)

5.1.3 Report on the Mini-Colloquium “Wide Bandgap Semiconductors”

CMD19/CMMP2002 Conference 2002
Brighton 7-11 April 2002

Sponsored by
European Science Foundation “Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces” (Psi-k)

Organized by
W. Richter (TU-Berlin, Germany) and J. Neugebauer (FHI-Berlin, Germany)

The mini-colloquium ”Wide bandgap semiconductors” at the CMD19/CMMP2002 meeting, organized by Prof. W. Richter (TU-Berlin, Germany) and Dr. J. Neugebauer (FHI-Berlin, Germany) covered advances in basic science issues as well as in novel applications of wide bandgap semiconductors. The 2 invited and 4 contributed talks covered various materials systems (group-III nitrides, SiC, group-II oxides) and addressed various materials related issues such as native point and extended defects, dopants, surfaces, device structures. For a brief summary of the invited talks see the abstracts below.

J. Neugebauer

Defects and doping in wide-band-gap semiconductors

C. G. Van de Walle

Xerox Palo Alto Research Center, USA

Lack of control over the conductivity of wide-band-gap semiconductors still presents a serious obstacle to device performance. After describing the first-principles approach we have developed to address these problems, I will focus on three issues: acceptor doping of nitrides, conductivity control in ZnO, and the role of hydrogen in dopant engineering of semiconductors in general. p-type doping of nitrides still relies entirely on magnesium. Our investigations indicate that beryllium could be a promising alternative, provided compensation can be brought under control. I will describe strategies for achieving this, including codoping with hydrogen. When H is incorporated, acceptor-hydrogen complexes are formed, and their detection forms a powerful means of monitoring the activation process. We have studied these complexes in detail, and identified a novel configuration of the Mg-H complex that exhibits some very unusual behavior in terms of low-energy excitations and the resulting entropy. Turning to ZnO, I will summarize the current understanding about the source of unintentional n-type conductivity, and the prospects for achieving p-type doping. Finally, since hydrogen plays an important role in many of these phenomena, I will discuss the electronic behavior of hydrogen in semiconductors and oxides in

general. Our initially surprising discovery that hydrogen acts as a donor in ZnO and in InN can actually be consistently explained in this broader context.

This work was supported in part by AFOSR (Contract No. F4920-00-C-0019) and by the Alexander von Humboldt Foundation. I gratefully acknowledge the hospi-tality of the Paul-Drude-Institut and the Fritz-Haber-Institut, Berlin.

Sensitive Electrons in Wide Bandgap Semiconductors

O. Ambacher, M. Eickhoff, C. E. Nebel, M. Stutzmann

Technische Universität München, Germany

Due to recent advances in their preparation and chemical manipulation, wide bandgap materials such as SiC, diamond, or the III-nitrides (GaN and AlGaN) have evolved into a distinct class of semiconductors with a large variety of new applications. The precise control of electronic and optical properties by substitutional doping, heteroepitaxy, and interface chemistry have already allowed the fabrication of superior electronic devices such as high efficiency blue LEDs and high power/high frequency oscillators, amplifiers, or integrated circuits. In addition, most wide bandgap semiconductors also feature excellent thermal, mechanical, and chemical stability, which makes this class of materials equally attractive for a wide range of applications in sensors, actuators, and for micro-electromechanical systems (MEMS). Of particular interest for sensor applications are the two-dimensional electron or hole gases (2DEGs or 2DHGs) which are obtained very close to the free surface of hydrogen-terminated diamond or GaN/AlGaN-heterostructures. The purpose of this talk is to discuss the present understanding of how such surface- or interface-related electronic systems come about, and to show how these can be put to good use for the sensitive detection of a surprisingly large number of external physical quantities.

5.1.4 Report on the Mini-Colloquium "Electronic Structure of Correlated Systems"

CMD19/CMMP Conference 2002
Brighton 7-11 April 2002

Sponsored by
European Science Foundation "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" (Psi-k)

Organized by
W.M. Temmerman (Daresbury), A. Georges (Paris), and T. Pruschke (Augsburg)

The Mini-Colloquium "Electronic Structure of Correlated Systems" consisted of one invited talk, whose abstract is given below, four contributed talks and 15 posters. The invited talk was by Sasha Lichtenstein on **"Realistic description of strongly correlated materials"**, utilising the dynamical mean field theory (DMFT) in conjunction with LDA, the so-called LDA+DMFT. Sasha showed how to go beyond the local spin density approximation and include spin and charge fluctuations with the DMFT. The central objects of the presented results were the spectral functions. These allow to make direct contact with photoemission data, which the speaker did quite succesfully. The contributed talks were by:

J. Bünemann (*Oxford*), F. Gebhard (*Marburg*), W. Weber (*Dortmund*), R. Claessen (*Augsburg*), V. Strocov (*Augsburg*) on **"Quasi-particle dispersion in nickel: progress in theory and experiment"**. In this talk the Gutzwiller-DFT was used to obtain satisfactory with experimental data, in particular the correct topology of the nickel Fermi surface, and to explain small but rather anisotropic exchange splitting of the bands.

L. Petit (*Aarhus*), A. Svane (*Aarhus*), W.M. Temmerman (*Daresbury*), Z. Szotek (*Daresbury*) on **"Ab-initio study of the localized-delocalized $5f$ transition in the UPd_3-UPt_3 system"**. In this talk the self-interaction corrected (SIC)-LSD method was applied to describe the electronic structure of URh_3, UPd_3,UPt_3,and UAu_3, providing a consistent description of both itinerant and localized $f-$electrons in these systems. Also, the calculated valencies are in good agreement with experiments, and UPt_3 is predicted to represent a high pressure phase of isoelectronic UPd_3.

K. Held (*Princeton*), G. Keller (*Augsburg*), V. Eyert (*Augsburg*), D. Vollhardt (*Augsburg*), V.I. Anisimov (*Ekaterinburg*), A.K. McMahan (*Livermore*), R.T. Scalettar (*Davis*) on **"Realistic calculations of correlated electron systems with LDA+DMFT(QMC): From V_2O_3 to Ce"**. In this talk, the LDA+DMFT results are presented for V_2O_3 and Ce, employing the quantum Monte Carlo (QMC) technique to solve the DMFT single site problem. At finite temperatures, the results yield a disappearance of the quasiparticle resonance in both systems.

S. Biermann (*Paris*), A.I. Lichtenstein (*Nijmegen*), M. Katsnelson (*Ekaterinburg*) on **"Hubbard bands in $\gamma-$manganese"**. In this talk the results for spectral properties of $\gamma-$manganese obtained with LDA+DMFT were presented. The results show good agreement wit recent experiments, proving importance of correlation effects in a seemingly simple transition metal.

The minicolloquium was rounded off with a quite successful poster session, highlighting the usefulness of band theory, and enhanced band theory in the understanding of the electronic and magnetic proprties of correlated electron systems.

Walter M. Temmerman

REALISTIC DESCRIPTION OF STRONGLY CORRELATED MATERIALS

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Local density approximation (LDA) for the electronic structure calculations has been highly successful for non-correlated systems. The LDA scheme quite often failed for strongly correlated materials containing transition metals and rare-earth elements with complicated charge, spin and orbital ordering. We discuss recent progress beyond the static density functional approximation, which includes finite temperature effects related to the charge, spin and orbital fluctuations in a self-consistent manner. Dynamical mean field theory (DMFT) in combination with the first-principle LDA scheme (LDA+DMFT) can be a starting point for the construction of a new spectral density functional for a realistic description of various correlated electron materials.

5.1.5 Report on the Mini-Colloquium "Non-Collinear Spin Structures"

CMD19/CMMP Conference 2002
Brighton 7-11 April 2002

Sponsored by
European Science Foundation "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" (Psi-k)

Organized by
J. Hafner (Wien), S. Blügel (Juelich), L. Nordström (Uppsala)

The minicolloquium consisted of 2 invited papers by G. Bihlmayer and M. Marsman and 3 contributed ones by E. Sjöstedt, L.M. Sandratskii and L.A. Prozorova. The five abstracts are attached. In addition there were eight poster contributions.

Ab-initio prediction of complex magnetic structures in low dimensions

G. Bihlmayer, Ph. Kurz, S. Blügel*
Forschungszentrum Juelich, Germany
**Universitaet Osnabrueck, Germany*

An accurate and realistic description of magnetic systems requires ab-initio methods that are able to handle non-collinear magnetic structures. Within the vector spin-density formulation of density functional theory we developed a program, FLEUR, that allows us to deal with (i) arbitrary commensurate spin-structures by employing a (intra-atomic non-collinear) constraint-field, (ii) incommensurate spin-spirals and (iii) the relaxation of the spin directions. This massively parallelized program is based on the full-potential linearized augmented planewave (FLAPW) method for bulk- and film geometry. In this method it is possible to accurately describe a wide variety of systems with open structures and low symmetry. Force calculations allow to determine simultaneously the magnetic and structural ground state. The direct access to exchange coupling constants via calculations with constrained spin directions opens up the possibility of a systematic approach to the investigation of the magnetic ground-state of a system by the combination of these ab-initio calculations with model Hamiltonians. We apply this technique to transition metals on a triangular lattice where a new magnetic ground state for the Mn/Cu(111) system has been found [1]. We show how to simulate finite temperature effects with spin-spiral calculations in a frozen-magnon model for the example of the Gd(0001) surface. The modeling of domain walls in thin films can be accomplished by combination of non-collinear calculations and the determination of the magnetocrystalline anisotropy energy. We present first results for Fe overlayers on W(110).

[1] Ph. Kurz, G. Bihlmayer, K. Hirai and S. Blugel, Phys. Rev. Lett. **86**, 1106 (2001).

Ab initio density-functional studies of noncollinear magnetism

M. Marsman, D. Hobbs, G. Kresse, J. Hafner
Universitaet Wien, Austria

In recent years much interest has been directed towards noncollinear magnetism, i.e., magnetic structures in which the magnetization density is a continuous vector variable of position, instead of being constrained to a global quantization axis. The technique to deal withfully unconstrained-noncollinear magnetism, within the framework of the projector augmented wave method, has been implemented in the Vienna Ab initio Simulation Package (VASP). We present the results of calculations on the incommensurate spin spiral ground state of bulk γ-Fe focussing on aspects of its structural stability, and the (preliminary) results of our investigations into the occurence of noncollinear spin arrangements in Fe monolayers grown on Cu(100) surfaces. We will furthermore illustrate the importance of the concomitant optimization of aspects of the crystalline structure and the spin system for complex magnetic systems, by way of our calculations on noncollinear magnetic states in α-Mn.

Full potential studies of non-collinear states in γ-Fe

E. Sjöstedt, L. Nordström
Uppsala University, Sweden

Accurate density functional calculations have been performed for the fcc-based frustrated antiferromagnet γ-Fe. Several competing collinear as well as non-collinear magnetic structures have been considered; ferromagnetism, lk, 2k, 3k, double layered type-I antiferromagnetism, as well as non-commensurate helices. In contrast to standard noncollinear methods, our scheme treats the magnetization density as a vector field which is free to change both in magnitude and direction throughout space. The non-collinear method is implemented in the alternative linearization of the the full-potential augmented-plane-wave method (FPAPW+lo), closely related to the conventionally linearized method (FLAPW), but computationally more efficient. The calculated groundstate of γ-Fe is found to vary sensitively with volume, going from a double layered anti-ferromagnetic structure to different helices as the volume is decreased. The ground state is found to be almost degenerate between two different helices having different equilibrium volumes. The obtained results are analyzed and compared with earlier calculations and existing experiments. For instance, we notice that the results are altered when we introduce an atomic moment approximation in our calculations.

Spin wave dispersion and Curie temperature in YFe_2 and UFe_2

L.M. Sandratskii, L. Bergqvist*, O. Eriksson*, P Bruno
Uppsala University, Sweden

Inelastic neutron diffraction experiment [1] revealed a number of unusual features in the properties of YFe_2 and UFe_2. The first feature is the absence of any observable mode involving the Y and U states. Second, the Fe-Fe exchange interaction as judged by the dispersion of the Fe mode is very strong. The parameter of the exchange interaction deduced from the value of the exchange stiffness in YFe_2 is very close to the value for bcc-Fe whereas for UFe_2 it is 5 times higher than for bcc-Fe. However, the value of the Curie temperature in UFe_2, 165 K, is low and is much smaller than the value of the Curie temperature in YFe_2, 545 K, or in bcc-Fe, 1043 K. We report parameter-free calculation of the spin-wave dispersion in YFe_2 and UFe_2. We show that though no inelastic scattering is detected from the Y and U cites the behavior of the magnetic moments of these atoms influences strongly the form of dispersion curve. For YFe_2 we get good agreement with the experiment in the whole energy region of magnon excitations reported. For UFe_2 we get good agreementwith experiment in the low energy region (large spin stiffness) but strong softening of magnons in higher energy region. Exchange interactions in the system are discussed and relation between magnon softening and low Curie temperature in UFe_2 is studied.

[1] L. Paolasini et al., Phys. Rev. B **59**, 6867 (1999).

Triangular lattice antiferromagnet, $RbFe(MoO_4)_2$, in an applied magnetic field

L. A. Prozorova, L. E. Svistov, A. I. Smirnov, O. A. Petrenko*, L. N. Demianetst, A. Ya. Shapiro†
P.L. Kapitza Institute for physical problems RAS, Russia
**University of Warwick, United Kingdom*
†*A.V. Subnikov Institute of Crystallography RAS, Russia*

$RbFe(MoO_4)_2$ is a rare example of a nearly two dimensional Heisenberg antiferromagnet on a triangular lattice. We have studied its low-temperature magnetic properties by means of single crystal ESR spectroscopy and magnetization measurements. On the basis of the obtained results an H-T phase diagram, containing at least five different magnetic phases is reproduced. In zero field, $RbFe(MoO_4)_2$ undergoes a phase transition at $T_N = 3.8$K into a noncollinear spin structure with all the spins confined in the hexagonal plane. The application of an external magnetic field in the plane induces a collinear spin state ($H_{C1} = 4.7$T, $H_{C2} = 7.1$T) and produces magnetization plateaux at one third of the saturation moment in agreement with previous powder magnetization data [1] and theoretical predictions [2]. Both the ESR and magnetization measurements also clearly indicate an additional first order phase transition in a field of 3.7T. The exact nature of this phase transition is unclear, although it is likely to be related to the presence of the incommensurate magnetic order, which was detected recently by neutron diffraction measurements [3].

[1] T. Inami, Y. Ajiro and T. Goto, J. Phys. Soc. Japan **65**, 2374, 1996.

[2] A.V. Chubukov and D.I. Golosov, J. Phys.: Cond. Matt. **3**, 69, 1991.

[3] C. L. Broholm, private communication.

5.1.6 Report on PHYSICS OF MAGNETISM'02 Conference

The European Conference
PHYSICS OF MAGNETISM'02
1-5 July, 2002 Poznań, Poland

Report on the European Conference *Physics of Magnetism'02*

Sponsored by the European Science Foundation

Organised by
Andrzej Jezierski
Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
Roman Micnas
Institute of Physics, Adam Mickiewicz University, Poznań, Poland

The European Conference Physics of Magnetism'02 took place in Poznań, Poland from 1-5 July 2002. The Conference was the tenth of the series organised every three years since 1975 jointly by the Institute of Molecular Physics Polish Academy of Sciences and the Institute of Physics Adam Mickiewicz University.

The Conference was as an international forum for presentation and discussion of novel scientific ideas in a field of magnetic phenomena with special emphasis of the following subjects:

-novel metallic oxides and anomalous magnetoresistive materials

-low dimensional quantum magnets

-heavy fermions, fluctuating valence and Kondo systems

-magnetic multilayers, surfaces and nanostructures

-high temperature superconductors

-electronic structure by *ab–initio* methods

The main objective of the Conference was to bring together scientists and technologists from the Western, Central and Eastern European countries involved in research and applications of new magnetic materials and high temperature superconductors. 232 researchers from 22 countries spent five days discussing physics of new magnetic materials.

The plenary talks were presented by 24 invited scientists: 4 from Poland, 6 from USA, 8 from Germany, 1 from Czech Republic, Slovakia, Switzerland, France, the Netherlands and England.

Programme of the Conference consisted of plenary talks and contributed papers presented in oral form or as posters.

The proceedings containing plenary and selected papers will be published as a regular issue of *physica status solidi.*

During the Conference we celebrated the 50^{th} anniversary of the Polish Academy of Sciences.

It was important that the part of participants was PhD students and post docs from ab–initio group whose stay was supported by ESF.

The full list of participants and all abstracts are provided on the website

http://www.ifmpan.poznan.pl/zp2/pm02.html

Andrzej Jezierski (Poznań)

SCHEDULE

Monday, July 1

14^{45}-15^{00} OPENING

A. Jezierski, R. Micnas

I.1 SPIN DYNAMICS AND SPIN DEPENDENT TRANSPORT

Chairmen: A. Jezierski, R. Micnas

15^{00}-15^{35} **P.E. Wigen** *(invited speaker)*

Department of Physics, Ohio State University, Columbus, Ohio, USA

Ferromagnetic Resonance Force Microscopy: Probing Ferromagnets at the Micron Level

15^{35}-16^{10}**J. Barnaś** *(invited speaker)*

Institute of Physics, Adam Mickiewicz University and Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Spin Related Phenomena in Transport Properties of Magnetic Mesoscopic Systems

16^{10}-16^{30}**S. Krompiewski**

Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Effect of Contact Interfaces on Quantum Conductance of Armchair Nanotubes

16^{30}-17^{00}coffee break

I.2 ASPECTS OF MAGNETIC INTERACTIONS

Chairman: J.A. Morkowski

17^{00}-17^{35}**I. Turek** *(invited speaker)*

Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

Ab initio Theory of Exchange Interactions in Itinerant Magnets

17^{35}-18^{10}**I. Škorvanek** *(invited speaker)*

Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia

Soft Magnetic Nanocrystalline Materials: Intergrain Coupling and Spin Freezing

18^{10}-18^{45}**W. Nolting** *(invited speaker)*

Humboldt-Universität zu Berlin, Berlin, Germany

Kondo-Lattice Model: Application to Thin Ferromagnetic Local-Moment Films

19^{00}- GET TOGETHER PARTY

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Tuesday, July 2

II.1 MOSTLY RARE-EARTH SYSTEMS

Chairman: L. Kowalewski

9^{00}- 9^{35}**A. Simon** *(invited speaker)*

Max Planck Institute, Stuttgart, Germany

Magnetism in Low-Dimensional Compounds of Rare Earth Metals

9^{35}-10^{10}**P.Wachter** *(invited speaker)*

Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

Magnetism and Electronic Structure of Actinide Chalcogenides

10^{10}-10^{30}**A. Ślebarski**

Institute of Physics, University of Silesia, Katowice, Poland

Non-Fermi Liquid Behavior in CeRhSn

10^{30}-11^{00}coffee break

II.2 MOSTLY NON-FERMI LIQUID SYSTEMS

Chairman: R. Troć

11^{00}-11^{35}**B. Andraka** *(invited speaker)*

Florida University, Gainesville, USA

Non-Fermi Liquid Behavior in UCu_4Pd and Related Alloys

11^{35}-12^{10}**D. Kaczorowski** *(invited speaker)*

W. Trzebiatowski Institute for Low Temperature and Structure Research,

Polish Academy of Sciences Wrocław, Poland

Unusual Features of Itinerant Antiferromagnetism in UGa_3

12^{10}-12^{15} break

II.3 MOSTLY MAGNETIC MULTILAYERS

Chairman: H. Szymczak

12^{15}-12^{50}**K. Baberschke** *(invited speaker)*

Freie Universität Berlin, Berlin, Germany

Ferromagnetic Monolayers: A Fresh Look at Fundamentals

12^{50}-13^{20}**ORAL SESSION I**

1. M. Żołądź, **T. Stobiecki***, M. Otto and Röll

* Department of Electronics, University of Mining and Metallurgy,

Kraków, Poland

Domain structures of ferromagnetically coupled $(Fe_{97}Al_3)_{85}N_{15}/Al_2O_3$ multilayers

2. **M. Reiffers***, B. Idzikowski, S. Ilkovi, K.-H. Müller

* Institute of Experimental Physics, Slovak Academy of Sciences,

Košice, Slovakia

Electron-quasiparticle interaction in the melt-spun cubic $RECu_5$ (RE - heavy rare earths)

13^{20}-15^{30}lunch break

II.4 RARE-EARTH SYSTEMS, QUANTUM CRITICAL POINTS

Chairman: W. Suski

15^{30}-16^{05}**J.K. Freericks** *(invited speaker)*

Georgetown University, Washington, USA

Theoretical Description of the High-Temperature Phase of Yb and Eu Intermetallics

16^{05}-16^{40}**G. Borstel** *(invited speaker)*

Department of Physics, Osnabrück University, Osnabrück, Germany

Modeling of Defects and Surfaces in Perovskite Ferroelectrics

16^{40}-17^{10}coffee break

II.5 MOSTLY ELECTRONIC STRUCTURE: FIRST PRINCIPLE METHODS

Chairman: L. Wojtczak

17^{10}-18^{25}ORAL SESSION II

1. **J. Y. Rhee***, Yu. V. Kudryavtsev, K. W. Kim, and Y. P. Lee

* Department of Physics, Hoseo Univiversity, Asan, Choongnam, Korea

Electronic structures and various physical properties of Ni_3Al alloy

2. **J. Toboła***, S. Kaprzyk, P. Pecheur

* Faculty of Physics and Nuclear Techniques, University of Mining and Metallurgy, Kraków, Poland

Theoretical search for magnetic half-Heusler semiconductor

3. **A.R. Ferchmin*** and H. Puszkarski

* Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Surface resonance modes in magnetic nanoparticles: size scaling of the frequency versus surface anisotropy

4. **M. Zwierzycki***, K. Xia, P.J. Kelly, G.E.W. Bauer, I. Turek

* Faculty of Applied Physics and MESA, University of Twente, The Netherlands and Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Spin-injection through an Fe/InAs Interfaces

5. **Nic Shannon***

* Max Planck Institute, Dresden, Germany

Quantum and thermal effects in the double exchange ferromagnet

19^{30}– RECEPTION PARTY

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Wednesday, July 3

III.1 THEORY

Chairman: B. Fechner

9^{00}- 9^{35}**C. Lacroix** *(invited speaker)*

Laboratoire Louis Néel, CNRS, Grenoble, France

2D and 3D Spin Liquids in Frustrated Systems

9^{35}-10^{10}**K.I. Wysokiński** *(invited speaker)*

M. Curie-Skłodowska University, Lublin, Poland

Spin Triplet Superconductivity in Sr_2RuO_4

10^{10}-10^{30}**I. Eremin**

Institut für Teoretische Physik, Freie Universität, Berlin, Germany

Normal State Spin Dynamics in Sr_2RuO_4:

Anisotropy Due to Spin-Orbit Coupling

10^{30}-11^{00}coffee break

III.2/III3

MAGNETIC SEMICONDUCTORS/

THIN FILMS AND NANOSTRUCTURES

Chairman: R. Gałązka

11^{00}-11^{35}**T. Story** *(invited speaker)*

Institute of Physics, Polish Acad. of Sciences, Warsaw, Poland

Semiconductor EuS-PbS Ferromagnetic Multilayers

11^{35}-12^{10}**S.C. Erwin** *(invited speaker)*

Naval Research Laboratory, Washington DC, USA

Self-Compensation and Ferromagnetism in Mn-Doped GaAs

12^{10}-12^{45}**G. Reiss** *(invited speaker)*

University of Bielefeld, Bielefeld, Germany

Magnetoelectronic Properties of Thin Film Systems and Nanostructures

12^{50}-14^{40}lunch break

III.4 ORBITAL ORDERING IN MAGNETIC INSULATORS

Chairman: P. Wachter

15^{30}-16^{05}**B. Keimer** *(invited speaker)*

Max Planck Institute, Stuttgart, Germany

Spin Dynamics in Orbitally Degenerate Magnetic Insulators

16^{05}-16^{40}**A.M. Oleś** *(invited speaker)*

Marian Smoluchowski Institute of Physics, Jagiellonian University,
Kraków, Poland

Orbital Ordering and Fluctuations in Transition Metal Oxides

16^{40}-17^{10}coffee break

17^{10}-19^{10}**POSTER SESSION I** (P-3-01÷54; P-4-01÷39; P-5-01÷27)
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Thursday, July 4

IV.1 STRONGLY CORRELATED ELECTRON SYSTEMS

Chairman: A.M. Oleś

9^{00}- 9^{35}**R. Zeyher**

Max Planck Institute, Stuttgart, Germany

Competition Between Superconductivity and the Pseudogap Phase in the t-J Model

9^{35}-10^{10}**W. Temmerman** *(invited speaker)*

Daresbury Laboratory, Daresbury, Warrington, U.K.

Band Theory of Correlated Electron Systems

10^{10}-10^{30}**P. Wróbel**

W. Trzebiatowski Institute for Low Temperature and Structure Research,

Polish Academy of Sciences Wrocław, Poland

Excitons in the Upper Hubbard Band

10^{30}-10^{55}coffee break

10^{55}-12^{10}**ORAL SESSIONS: IIIa and IIIb**

ORAL SESSION IIIa

Chairman: A. Szytuła

1. **E. E. Kaul***, C. Geibel, A. V. Mironov, R. V. Shpanchenko
and E. V. Antipov
* Max-Planck Institut für Chemische Physik fester Stoffe,Dresden, Germany
Synthesis, structure and magnetic properties of $Pb_2VO(PO_4)_2$***: the second example for a frustrated S=1/2 square lattice antiferromagnet***

2. **T. Cichorek***, R.Wawryk, A. Wojakowski, Z. Henkie,
J. Custers, P. Gegenwart, F.Steglich, E.D. Bauer and M.B. Maple
* Max Planck Institute for the Chemical Physics of Solids, Dresden, Germany
and Institute of Low Temperature and Structure Research,
Polish Academy of Sciences, Wrocław, Poland
Interaction between tls and conduction electrons in actinide arsenoselenides

3. **V.H. Tran***, R. Troć, G. André and F. Bouré
* Institute of Low Temperature and Structure Research,
Polish Academy of Sciences, Wrocław, Poland
Ferromagnetic ordering in $UFe_{0.5}Ni_{0.5}Al$

5. **R. Puźniak***, M. Angst, A. Wiśniewski, J. Jun,
S.M. Kazakov, J. Karpinski, J. Roos and H. Keller
*Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
Evidence for a temperature and field dependence of

***the anisotropy of superconducting MgB**$_2$*

ORAL SESSION IIIb

Chairman: J. Baszyński

1. **S. Lipiński***, B.R. Bułka, W. Babiaczyk

* Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Coherent electronic transport through magnetic double tunnel junction

2. **Y. Kakehashi***

* Max-Planck Institut für PKS, Dresden, Germany

Dynamical CPA theory of magnetism

3. **I. Laulicht***, E. Sloutskin and S.R. Bishop

* Department of Physics, Bar-Ilan University, Ramat-Gan, Israel

The dependence of the auto-oscillation frequency of parametric spin-waves on the pumping power and inter mode interaction strengths

4. **V.K. Dugaev***, V.I. Litvinov, J. Barnaś, H. Slobodskyy,W. Dobrowolski, M. Vieira

* ISEL-DEETC, Lisbon, Portugal

Ferromagnetism in diluted magnetic semiconductors at low carrier density

5. **B.N. Filippov***

* Institute of Metal Physics, Ekaterinburg, Russia

Nonlinear dynamics of vortex-like domain walls in magnetic films with in-plane anisotropy (in russian)

12^{10}-12^{15}break

12^{15}-13^{30}**ORAL SESSIONS: IVa and IVb**

ORAL SESSION IVa

Chairman: B. Bułka

1. **T. Sakai***, N. Okazaki, K. Okamoto, K. Kindo,
Y. Narumi, Y. Hosokoshi, K. Kato, K. Inoue
* Department of Physics, Tohoku University, Sendai, Japan
Magnetization plateaux in S=1 spin ladder

2. **T. Roscilde***, A. Cuccoli, V. Tognetti, P. Verrucchi, R. Vaia
* Dipartimento di Fisica "A. Volta" dell'Universita di Pavia and INFM,
Pavia, Italy
Phase transitions and crossovers in anisotropic two-dimensional quantum antiferromagnets

3. N.A. Babushkina, **G.E. Fedorov***, A.V. Inyushkin, A.N. Taldenkov
* Institute of Molecular Physics,
Russian Research Centre - *Kurchatov Institute*, Moscow, Russia
Oxygen-isotope effect on magnetic properties of $Pr_{0.7}Ca_{0.3}MnO_3$ under strong pulsed magnetic fields

4. **G. Musiał***, L. Dębski, G. Kamieniarz
* Institute of Physics, Adam Mickiewicz University, Poznań, Poland
Monte Carlo simulations of the 3d Ashkin-Teller model: continuous phase transition lines

ORAL SESSION IVb

Chairman: Z. Jacyna-Onyszkiewicz

1. **U. Kuhlmann***, C. Thomsen, A.V. Prokofiev, F. Büllesfeld, E. Uhrig,
M. Anton, C. Gross and W. Assmus
* Institut für Festkörperphysik, Technische Universität Berlin,
Berlin, Germany
Magnon-phonon interaction in $(VO)_2P_2O_7$studied by Raman scattering

2. **N. Sluchanko***, V. Glushkov, S. Demishev, L. Weckhuysen,
V. Moshchalkov, A. Menovsky
* General Physics Institute of Russian Academy of Sciences, Moscow, Russia
Strong Hubbard correlations and weak magnetism in FeSi

3. **A. Lehmann-Szweykowska***, R.J. Wojciechowski, J. Barnaś,

P.W. Wigen

* A. Mickiewicz University, Institute of Physics, Poznań, Poland

Origin of the magnetoresistance in Ca-doped YIG

4. **A. Rogalev***, F. Wilhelm and J. Goulon

* European Synchrotron Radiation Facility (E.S.R.F.) Grenoble, France

Magnetism of anions: XMCD study

13^{40}-15^{30}lunch break

15^{30}-16^{15}**ORAL SESSION V**

Chairman: A. Sukiennicki

1. **G. Gubbiotti*** and L. Smardz

* Istituto Nazionale Fisica della Materia, Perugia, Italy

Exchange coupling in symmetric Co/Cr/Co trilayer:

a Brillouin light scattering study

2. **F. Wilhelm***, P.Poulopoulos, K. Baberschke and A. Rogalev

* European Synchrotron Radiation Facility (E.S.R.F.) Grenoble, France

Interface magnetism in 3d/5d multilayers probed by

X-ray magnetic circular dichroism

3. **J. Stankowski***, F. Stobiecki, M. Górska

* Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Application of magnetically modulated microwave absorption

to study GMR effect in Ni-Fe/Cu multilayer system

16^{15}-18^{15}

POSTER SESSION II (P-1-01÷38; P-2-01÷60; P-6-01÷17; P-7-01÷13)

bonfire

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Friday, July 5

V.1 High T_CSUPERCONDUCTORS

Chairman: S. Robaszkiewicz

9^{00}- 9^{35}**J. Zaanen** *(invited speaker)*

Lorentz Institute for Theoretical Physics, Leiden University,

Leiden, The Netherlands

Gauge Theory, Geometry and the Theory of Quantum Stripe Liquids

9^{35}-10^{10}**A. Bussman-Holder** *(invited speaker)*

Max Planck Institute, Stuttgart, Germany

Two-Component Scenario for Cuprates HTS with Mixed Order Parameters

10^{10}-10^{40}coffee break

Chairman: Y. Kakehashi

10^{40}-11^{15}**P. Coleman** *(invited speaker)*

Rutgers University, Piscataway, USA

How Does the Heavy Electron Decay at a Quantum Critical Point?

11^{15}-11^{35}**J. Haase**

Max Planck Institute for the Chemical Physics of Solids, Dresden, Germany

Spin and Charge Inomogeneity in the Cuprates Characterized by NMR

11^{35}-12^{05}SUMMARY (P.E. Wigen-experiment, J. Zaanen-theory)

12^{05}CLOSING

12^{30}LUNCH

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PM'02 – INVITED LECTURES

NON-FERMI LIQUID BEHAVIOR IN UCu_4Pd AND RELATED ALLOYS

Bohdan Andraka

Department of Physics, University of Florida P.O. Box 118440, Gainesville, FL 32611-8440, USA

UCu_4Pd is one of the first reported canonical non-Fermi liquid systems. Despite extensive research, the ground state properties of this compound and related $UCu_{5-x}Pd_x$ alloys is poorly understood. It is fair to say that neither of theoretical scenarios proposed accounts for the whole spectrum of unique properties of this solid. Among the intriguing and important questions we address is the persistence of non-Fermi liquid like behavior over extended range of concentrations x and strong sensitivity of UCu_4Pd to preparation conditions.

FERROMAGNETIC MONOLAYERS: A FRESH LOOK AT FUNDAMENTALS

Klaus Baberschke

Institut für Experimentalphysik, Freie Universität Berlin,
Arnimallee 14, D-14195 Berlin-Dahlem, Germany

Ultrathin ferromagnetic films of Fe, Co, Ni, etc. allow manipulations of the magnetism which are hardly accessible in the bulk : (i) Due to special growth mechanisms crystallographic structures can be prepared which are impossible in bulk magnetism, e.g. tetragonal Ni single crystals. (ii) As a consequence of the finite size effect one can shift the phase transition temperature T_{C} to almost any value between zero and the bulk Curie-temperature. (i) Changes of the c/a-ratio by a few percent or ≈ 0.05 Å of the nearest neighbor distance will change the magnetic anisotropy energy by $10^2 - 10^3$! This dramatic change is caused by the reactivation of orbital magnetism, being not anymore quenched like in bulk cubic ferromagnets. Experimental examples will be given which agree perfectly with ab-initio theory if the input parameter for ab-initio calculations are the real structures and not idealized fcc-, bcc-lattices. (ii) The thickness dependence of T_{C} is used to study the magnetic phase transition and the interlayer exchange coupling in a trilayer of Co/Cu/Ni. Separate $T_{\mathrm{C}}^{\mathrm{Ni}}$ and $T_{\mathrm{C}}^{\mathrm{Co}}$ for a coupled trilayer are observed and the effect of enhanced spin fluctuations in two dimensions will be discussed. For such an exchange-coupled trilayer we find a very strong temperature dependence of $J_{\mathrm{inter}}(T)$. Finally, we will discuss the Curie-Weiss-law for thin Fe films and its critical exponent γ.

The work was supported by DFG, Sfb 290 and BMBF(05KS1 KEB4)

SPIN RELATED PHENOMENA IN TRANSPORT PROPERTIES OF MAGNETC MESOSCOPIC SYSTEMS

J. Barnaś[a,b]**, V. Dugaev**[c]**, J. Martinek**[b]**, W. Rudziński**[a]**,**
R. Świrkowicz[d]**, I. Weymann**[a]**, M. Wilczyński**[d]

[a] *Department of Physics, Adam Mickiewicz University, Poznań, Poland*
[b] *Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland*
[c] *Department of Electronics and Communications, ISEL, Lisbon, Portugal*
[d] *Faculty of Physics, Technical University, Warszawa, Poland*

Spin effects in transport properties of magnetic mesoscopic systems will be reviewed, with particular attention paid to new physical phenomena and their possible applications in magnetoelectronics/spintronics devices. This includes the phenomena which occur when electrons cross an interface between nonmagnetic and ferromagnetic systems, like for instance nonequilibrium spin accumulation, spin injection, and local torque acting on the system. In the latter case, the torque may lead to current-induced magnetization switching. Main emphasis, however, will be on spin polarized transport in double ferromagnetic junctions, including crossover from planar double-barrier junctions to double junctions with a single-level quantum dot as the central part. Owing to the tunnel magnetoresistance effect, such systems may be used in field sensors. Apart from this, they also can operate as magneticaly controlled single electron transistors, diodes, spin injectors, spin polarizers, etc. Some new physical phenomena, like for instance magneto-Coulomb oscillations, spin blockade, and others may also occur in these systems.

MODELING OF DEFECTS AND SURFACES IN PEROVSKITE FERROELECTRICS

Gunnar Borstel

Department of Physics, University of Osnabrueck,
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Thin ferroelectric films are important for the development of optical wave-guides and integrated optics applications. The $SrTiO_3$ (110) surface is also widely used as a substrate for the cuprate superconductor growth. It is well known that the efficiency of ferroelectric devices is strongly affected by the presence of point defects, first of all, vacancies which are always present in non-stoichiometric crystals. In this talk, we present the state-of-the art of computer modeling of perfect and defective bulk perovskites and their surfaces, combining quite different theoretical approaches ranging from first principles to semi-empirical quantum mechanical and classical shell-model methods. Among the topics treated are: F-type electron centers (O vacancy which trapped one or two electrons), hole polarons bound to a K vacancy, self-ordering effects, and surface relaxation for $SrTiO_3$ surfaces with different terminations.

HOW DOES THE HEAVY ELECTRON DECAY AT A QUANTUM CRITICAL POINT?

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A series of new experiments on quantum critical points [1] begin to give usnew insight into way the Fermi liquid evolves into a quantum criticalpoint, and the nature of the break-up of the heavy electron quasiparticleat the quantum critical point. This talk will discuss how the recentobservation of the constancy of the Kadawaki Woods [1] ratio in thefield-tuned approach to a QCP indicates that the underlying scatteringamplitudes are renormalized in energy, but contain no strong momentumdependence. This discovery definitively rules out a spin density wavescenario for the heavy fermion QCP. The talk will will discuss scenarioswhere a complete break-up of the heavy electron quasiparticle leads to ajump in the Hall constant at the heavy electron quantum critical point, and will outline the constraints this places on a future theory of this phenomenon.

[1] J. Custers, P. Gegenwart et al. , to be published.

SELF-COMPENSATION AND FERROMAGNETISM IN Mn-DOPED GaAs

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Ferromagnetism in Mn-doped GaAs is generally believed to be mediated by holes arising from substitutional Mn. Measured hole concentrations are much smaller than expected from simple electron counting, for unknown reasons. We present theoretical evidence that the source of this compensation is interstitial Mn. We show that under non-equilibrium conditions characteristic of the low temperatures used during growth, interstitial Mn can be formed by a simple low-energy surface adsorption process. In the bulk, interstitial Mn plays a dual role: as a source of hole compensation, and as a source of localized spins whose interactions are mediated by electrons. We develop a mean-field theory of magnetism that self-consistently accounts for both substitutional and interstitial Mn as well as their mutual compensation.

THEORETICAL DESCRIPTION OF THE HIGH-TEMPERATURE PHASE OF Yb AND Eu INTERMETALLICS

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A number of different Yb and Eu intermetallic compounds (such as $\mathrm{YbInCu_4}$ and $\mathrm{EuNi_2(Si_{1-x}Ge_x)_2}$) display anomalous behavior as a function of temperature. At high temperature, the systems possess local moments with a Curie-like susceptibility and show no signals of the Kondo effect. They appear to be "dirty" metals with unscreened local moments and large thermopower. As the temperature is lowered, these systems undergo a transition to an intermediate-valence state, where the local moments are screened, and the number of charge carriers is increased. One way to describe these systems is via a combined periodic Anderson and Falicov-Kimball model. The system has the f-levels lying just above the chemical potential at zero temperature. In the high-temperature phase, the Kondo effect renormalizes to zero, and the local moments appear due to thermal activation. The system becomes more resistive due to the presence of a gap in the single-particle density of states. As temperature is lowered, a transition occurs to an intermediate-valence state with fully screened local moments. When we restrict the analysis to consider only the Falicov-Kimball model, then a finite-temperature crossover occurs between the high-temperature phase with many local moments to a low-temperature phase with no local moments. Much of the physics of these systems seems to be accounted for within this scenario, even though it does not properly capture the quantum-mechanical intermediate-valence low-temperature phase.

UNUSUAL FEATURES OF ITINERANT ANTIFERROMAGNETISM IN $\mathrm{UGa_3}$

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Antiferromagnetic UGa_3 is a prototypical representative of an unusual class of itinerant magnets with large orbital moments. Although the magnetic, electrical transport and thermodynamic properties of this compound closely resemble those of 3d-electron transition-metal systems, some peculiar features unambiguously manifest the presence of large orbital moments, as in lanthanide-based materials with localized 4f-electrons. This unique behavior of itinerant 5f-electrons makes UGa_3 an interesting system for both experimental and theoretical studies. In the talk, we shall review the results of a series of sophisticated experiments performed on high-quality single crystals of UGa_3: elastic and inelastic neutron scattering, optical ellipsometry, resonant X-ray magnetic scattering, Mössbauer spectroscopy. Among other topics we shall discuss a two-component dynamical magnetic response, related to fast and slow quasiparticle excitations in the ordered state, and a giant enhancement of the RXMS signal at the K-edge of nonmagnetic Ga anion, which possibly involves the hybridization of the gallium 4p-orbitals with the uranium 5f-states. The experimental findings will be compared to the calculated results, derived in the framework of local spin density functional theory.

*Work done in collaboration with M.M. Abd-Elmeguid, N. Bernhoeft, M.S.S. Brooks, A. Czopnik, A. Hiess, G. H. Lander, P.M. Oppeneer, J.P. Sanchez, J. Schoenes.

SPIN DYNAMICS IN ORBITALLY DEGENERATE MAGNETIC INSULATORS

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The interplay between spin and orbital degrees of freedom in transition metal oxides has been a subject of investigation since the 1950's. Recent advances in materials preparation have made it possible to go beyond the *static* spin and orbital arrangements that have been studied for many years, and to investigate the spin and orbital *dynamics* in d-electron systems. Because of the high orbital degeneracy and the weak lattice coupling, the coupled quantum dynamics of spins and orbitals is expected be particularly interesting for systems with partially occupied t_{2g} orbitals such as titanium and vanadium oxides. Indeed, we show that recent neutron scattering experiments on insulating versions of these systems are inconsistent with conventional models of orbital order in magnetic insulators. We discuss the outcome of these experiments and outline some steps towards a quantum many body description of the coupled spin and orbital dynamics of insulators with orbital degeneracy.

If time permits, we will also briefly discuss recent experimental progress on the spin dynamcis of the superconducting copper oxides.

* Collaboration with C. Ulrich, G. Khaliullin, J. Sirker, S. Okamoto, M. Reehuis, A. Ivanov, S. Miyasaka, Y. Taguchi, and Y. Tokura

MAGNETISM OF 2D AND 3D FRUSTRATED SYSTEMS

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In the last few years, new physics has been shown to occur in fully frustrated lattices such as Kagomé or pyrochlore lattices: various types of behaviors are obtained, depending on the details of interactions; a short review of the possible, and eventually observed in some compounds, ground states will be given: quantum spin 1/2 systems exhibit a quantum spin liquid ground state with a spin gap, but a continuum of low energy singlet states; classical spins do not order and the ground state is infinitely degenerate; effect of anisotropy is quite important and leads to spin-ice behavior; "order by disorder" due to quantum or classical spin fluctuations may occur in some cases. Moreover any small perturbation (for example dipolar interaction) may change completely the physics of the system. New results related to the effect of Dzyaloshinsky-Moriya interactions (DMI) will be presented. It will be shown that DMI are always allowed in these structures due to the low local symmetry; the effect on DMI on the ground state changes completely the nature of the ground state; magnetic ordering occurs due only to DMI. Possible application of the model to Fe and Cr jarosites with the kagom structure will be presented. This would be the 1^{st} example of a magnetic transition induced by DMI.

KONDO-LATTICE MODEL: APPLICATION TO THIN FERROMAGNETIC LOCAL-MOMENT FILMS

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We study correlation effects and temperature dependencies in the electronic structure of thin ferromagnetic local-moment films. In a first step the Kondo-lattice model is investigated as a candidate for a proper representation of local-moment ferromagnets. Magnetic and electronic key-quantities as the Curie-temperature and the quasiparticle density of states are derived with previously tested many-body procedures. It is shown that the magnetic properties can beinterpreted exclusively in terms of the temperature-dependent electronic quasiparticle structure. An extended RKKY theory leads to effective Heisenberg exchange integrals, which turn out to be functionals of the conduction electron selfenergy, getting therewith a remarkabletemperature and band occupation dependence. In a second step the model studies are combined with tight binding-LMTO bandstructurecalculations in order to get for real ferromagnetic films quasiparticle densities of states andquasiparticle bandstructures. The proposed method avoids the double-counting of relevantinteractions and takes into account the correct symmetry of the atomic orbitals. Special results are given for thin ferromagnetic EuO (100) films. The Curie temperatureT_C of the EuO film turns out to be strongly thickness-dependent, starting from a very lowvalue ($\simeq$ 15 K) for the monolayer and reaching the bulk value at about 30 layers. For a 20-layer film we predict the existence of a surface state, the temperature-behaviour of which can lead to a surface halfmetal-insulator transition.

ORBITAL ORDERING AND FLUCTUATIONS IN TRANSITION METAL OXIDES

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A short review of the frustrated magnetic interactions in transition metal oxides with orbital degrees of freedom is presented. The classical phase diagrams of e_g systems show a competition between different phases, with spin, orbital and mixed spin-and-orbital excitations, and strongly enhanced quantum fluctuations [1]. The orbital order explains a quasi-one-dimensional antiferromagnetic (AF) interactions of spins $S = 1/2$ in $KCuF_3$, and the measured superexchange between spins $S = 2$ in the A-AF phase of $LaMnO_3$. The spectral functions of a single hole in $LaMnO_3$ depend strongly on the type of the underlying orbital order [2]. Macroscopic hole doping $x \simeq 0.3$ promotes an orbital liquid in the ferromagnetic manganites, and the observed increase of the spin stiffness with x is well explained by e_g electron correlations [3]. Quantum fluctuations of t_{2g} orbitals play a prominent role in early transition metal oxides — they explain the isotropic AF order in $LaTiO_3$, and enhance ferromagnetic interactions in the C-AF phase of cubic vanadates. Finally, the t_{2g} orbital fluctuations stand behind the exotic magnetic properties of YVO_3, and stabilize the C-AF over G-AF order at finite temperatures [4].

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MAGNETOELECTRONIC PROPERTIES OF THIN FILM SYSTEMS AND NANOSTRUCTURES

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Following the discovery of the antiferromagnetic coupling of Fe layers via the conduction electrons of Cr in thin multilayered systems by Grnberg and the Giant MagnetoResistance by Fert, solid state researchers started to intensively explore the dependence of the electron transport and tunneling on the spin in thin film systems. This talk will first give an overview of the current status of this work on metallic multilayers and tunneling elements. The second part will concentrate on applications of these new devices and will give an outlook on new developments in magneto- and spinelectronics.

MAGNETISM IN LOW-DIMENSIONAL COMPOUNDS OF RARE EARTH METALS

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Metal-rich halides of rare earth elements lie on the borderline between salts and metals. They are particularly interesting due to the presence of localised or itinerant (d) electrons in low-dimensional bond systems together with localised (f) electrons. Out of a large body of new compounds and structures one- and two-dimensional systems are chosen to illustrate magnetic phenomena governed by d-d interaction, frustration effects etc. Special emphasis is given to 2 D metallic systems like GdI_2 which orders ferromagnetically at 290 K and exhibits GMR with a negative magnetoresistance of 70% at room temperature in a field of 7 T. Structures based on twin-layers of metal atoms allow extensive compositional variations with respect to the atoms placed between the twin-layers as will be discussed for the interstitials H, C and Fe. The hydride halides $LnXH_n$ offer a way to reversibly tune the (d) carrier density via the H content. For $n = 2$ they are insulators, and for $0.67 \leq n \leq 1.00$ the phases are metallic. Detailed investigations of the CE-type antiferromagnetism of $TbBrH_n$ are reported which becomes a spin glass at $n = 0.67$.

SOFT MAGNETIC NANOCRYSTALLINE MATERIALS: INTERGRAIN COUPLING AND SPIN FREEZING

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The reduction of the grain size to the nanometer range may vary drastically the physical properties of materials, including the magnetic behaviour. Typical examples of such systems are Fe–based extremely soft magnetic alloys. The macroscopic magnetic properties of these materials arise from the interplay of the microscopic parameters such as grain, size, intergrain coupling, anisotropy and interface effects. In this work, the static and dynamic properties of nanocrystalline soft magnetic alloys consisting of Fe–nanograins embedded in an amorphous matrix are investigated by means of dc and ac susceptibility, magnetization and hysteresis loop measurements in a wide temperature range. We show that some alloys of this group exhibit particular complex magnetic properties versus temperature. The spin–glass like behavior is observed at low temperatures. Here a remarkable magnetic anisotropy could be induced after cooling the samples though freezing temperature in an external magnetic field. These low temperature features are followed by very soft magnetic behaviour at intermediate temperature range, and finally, a marked magnetic hardening due to decoupling between the nanograins is observed when temperature approaches the Curie temperature of amorphous residual phase. Striking differences in the decoupling behaviour are observed and discussed for the samples with different volume fractions of nanocrystalline particles.

SEMICONDUCTOR EuS-PbS FERROMAGNETIC MULTILAYERS

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EuS-PbS multilayers constitute all-semiconductor ferromagnetic-nonmagnetic structures with magnetic layers of EuS (a model nonmetallic ferromagnet) and diamagnetic layers of PbS (the well known semiconductor compound with its energy gap in the infrared). As lattice parameters of EuS and PbS match very well the variety of epitaxial heterostructures can be grown by high vacuum deposition techniques. Ferromagnetic transition in EuS-PbS multilayers is observed even in the structures with ultrathin EuS layers of only 0.6 nm (2 monolayers). The Curie temperature depends on the thickness of the magnetic layer as well as on the strain generated because of the difference between the thermal expansion coefficients of the multilayer and the substrate. These effects will be discussed for the variety of EuS-PbS structures grown on various substrates: KCl (100), BaF_2(111) and PbS (100). For sufficiently thin (typically below 3 nm) nonmagnetic PbS spacer layers in EuS-PbS multilayers one observes pronounced magnetic effects related to the antiferromagnetic interlayer coupling between EuS layers. The experimental work as well as the physical mechanisms relevant for this effect will be discussed. Due to the large exchange splitting of the conduction band states in EuS the EuS-PbS multilayers form an intriguing spintronic system. Recent work concerning the tunneling structures exploiting spin filter effect will be reviewed as well.

BAND THEORY OF CORRELATED ELECTRON SYSTEMS

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A review will be given of the self-interaction corrected local spin density (SIC-LSD) method to describe the electronic and magnetic properties of strongly correlated d and f electron systems. Applications of the method for the determination of the valency of rare earths and actinides will be presented. Recent results on the metal/insulator transition in YBCO, half metallicity of Sr_2FeMoO_6 and orbital ordering in $LaMnO_3$ will be discussed.

AB INITIO THEORY OF EXCHANGE INTERACTIONS IN ITINERANT MAGNETS

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The lecture reviews an efficient two-step procedure to determine magnetic properties of itinerant magnets from first principles. In the first step, the selfconsistent electronic structure of a system is calculated using the tight-binding linear muffin-tin orbital method combined with Green function techniques, which is appropriate for description of substitutional randomness of disordered bulk alloys and for two-dimensional translational periodicity of layered systems like surfaces and thin films. In the second step, the parameters of the effective classical Heisenberg Hamiltonian are determined using the magnetic force theorem and they are employed in subsequent evaluation of magnon spectra, the spin-wave stiffness constants and the Curie temperatures. Examples of application include:

(i) ferromagnetic $3d$ metals Fe, Co, and Ni,

(ii) disordered transition-metal alloys like bcc Fe-Co,

(iii) ultrathin magnetic films of Fe and Co on a Cu(001) substrate,

(iv) diluted magnetic semiconductors (Ga,Mn)As, and (v) f-electron systems like hcp Gd.

The developed theory will be presented together with selected aspects of the numerical implementation and with a comparison to existing experimental data.

MAGNETISM AND ELECTRONIC STRUCTURE OF ACTINIDE CHALCOGENIDES

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The magnetism of the light actinide chalcogenides from U up to Am is largely determined by the electronic structure of these materials and the degree of f localization. The U chalcogenides are simple trivalent $5f^3$ ferromagnetic metals with eV wide 5f bands. The Np chalcogenides NpS and NpSe are trivalent, have a $5f^4$ configuration and they exhibit type II antiferromagnetic ordering. We still have a relatively wide 5f band and f-d hybridization. According to the Luttinger theorem materials with an odd f+d count, here 5, should not exhibit a hybridization gap. Nevertheless the resistivity shows activated behavior. A gap appears in an antiferromagnet with a magnetic unit cell twice the chemical cell and the f-d count is even again. Nonmagnetic NpTe indeed has no activated resistivity. The Pu chalcogenides are intermediate valent and with an even f-d count (6) they have hybridization gaps in the meV range and f band widths in the tens of meV. The magnetism is of the Pauli type but with an enormous susceptibility. Finally in AmTe we have a divalent $5f^7$ configuration, but with a narrow 24 meV half filled 5f band, it is thus a heavy fermion with $m^* \cong 330m$ and shows an even stronger Pauli susceptibility than PuTe. If the assignment is correct, 5f localization is not yet achieved in the Am chalcogenides but only in the Cm chalcogenides. Instead localization in the actinide metals is claimed already in Am.

PROBING FERROMAGNETS AT THE MICRON LEVEL*

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With the development of fabrication methods to produce materials and devices at nanoscale dimensions, there is a need for the development of new techniques to characterize the materials in new devices at these dimensions. In the field of magnetic materials these devices include spintronic elements and submicron magnetic memory storage elements. Magnetic Resonance Force Microscopy (MRFM) is a new technique first observed in 1992 and has the theoretical sensitivity of single spin detection and atomic resolution. MRFM combines the principles of magnetic resonance with those of scanned probe technology to detect spin resonance through mechanical, rather than inductive, means. This talk will review the recent progress in the field using both NMRFM and ESRFM. Ferromagnetic resonance force microscopy (FMRFM), a third variant of MRFM first demonstrated in 1996, is an application developed to investigate ferromagnetic samples. It enables (a) the characterization of the dynamic magnetic properties of magnetic structures at the *micron scale*, and (b) the spatial resolution of the ferromagnetic resonance mode within such samples. In addition the technique will (c) lead to the observation of localized resonances due to the strong perturbation of the probe magnet on the sample.

* This collaborative work is carried out jointly with Caltech (Roukes Group) and LANL (Hammel Group)

SPIN TRIPLET SUPERCONDUCTIVITY IN Sr_2RuO_4

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Sr_2RuO_4 is at present the best candidate of the solid state superconducting analogue of the triplet superfluidity in ^{3}He. The material is a good (albeit correlated) Fermi liquid in the normal state and an exotic superconductor below T_c. The mechanism of superconductivity and symmetry of the order parameter remain main puzzling issues of on-going research. In the talk I shall present the results of our search for the correct superconducting state realised in the material. Our calculations are based on a three-dimensional three-band effective model with a realistic band structure. We have found a state with non-zero order parameter at each of the three sheets of the Fermi surface. The corresponding gap in the quasiparticle spectrum has line or point nodes on the α and β sheets and is complex with no nodes at the γ sheet. This state describes remarkably well a number of existing experiments including power low temperature dependence of the specific heat, penetration depth, thermal conductivity etc. The stability of the state with respect to disorder and spin-orbit coupling will be also briefly analysed.

GAUGE THEORY, GEOMETRY AND THE THEORY OF QUANTUM STRIPE LIQUIDS

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A consensus has emerged that stripes are a generic phenomenon associated with the doped Mott-insulating state. The cuprate high Tc superconductors are special in the sense that the superconductivity goes hand in hand with the quantum-destruction of the static stripe phase. The question is, can this competition give rise to new states of quantum matter which cannot be reached by adiabatic continuation starting from a BCS superconducting state? In our way of thinking, the key property making stripes more than just charge and spin order is the empirical fact that the charge stripes are *Ising* domain walls in the spin system. Based on both emperical information and theoretical arguments, we claim that this 'antiphaseboundariness' acquires a life of its own as independent dynamical degree of freedom in the long wavelength realms. We demonstrate that this antiphaseboundariness is controlling the spin-charge separation of the one dimensional electron-Luttinger liquids; it is rooted in the 'squeezed space' *geometrical* structure discovered by Ogata and Shiba in the Bethe-ansatz solutions which can be linked to Z_2 gauge degrees of freedom. We promote this 1+1D vacuum structure to physical principle, to ask what happens when it is applied to 2+1 dimensions. When charge order takes over static stripes result. However, the charge disordered/superconducting phases are far more interesting. The rich physics of 2+1D Ising gauge theory switches on, and we predict a variety of novel phases like the quantum spin-nematic. Phases of this kind might be realized in the cuprates at intermediate dopings. Although it is impossible to measure the order parameters associated with these phases directly with existing experiments, we will present some indirect consequences which can be experimentally verified.

PM'02 – SELECTED (*ab–initio*) CONTRIBUTED PAPERS

NON-FERMI LIQUID BEHAVIOR IN CeRhSn

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Electrical resistivity ρ, magnetic susceptibility χ, specific heat C, X-ray photoelectron spectroscopy (XPS), and the calculations of the electronic structure were made on the compound CeRhSn. The data demonstrate the scaling behavior of the non-Fermi liquid; $C(T)/T \propto \chi \propto T^{-1+\lambda}$, and $\Delta\rho \propto T$. We argue that the non-Fermi liquid behavior observed in CeRhSn can be due to the existance of a Griffith's phase close to a quantum critical point.

SPIN-INJECTION THROUGH AN Fe/InAs INTERFACES

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Current interest in spin-injection into semiconductors is motivated both by the fundamental aspects of the phenomenon and by potential applications. The basic obstacle to spin-injection from a metallic ferromagnet into a semiconductor is the large difference in their conductivities; the resistivity of a semiconductor such as InAs is much larger than either the majority- or minority-spin resistivity of Fe. However, the spin-dependent interface resistance if sufficiently large could generate a spin-dependent potential drop at the interface. Here, we evaluate this term for an Fe/InAs interface from first principles. The formalism based on the tight-binding linear-muffin-tin orbital surface Green's function method allows us to treat large lateral superlattices so that we can study the influence of disorder on the conductance. We find that due to the symmetry mismatch in the minority-spin channel the specular interface acts as an efficient spin filter with the polarisation of transmitted current close to 100%. The resistance of a diffusive interface is comparable to the resistance of an InAs slab several hundreds nanometers thick but the symmetry breaking due to the disorder can substantially reduce the spin-asymmetry. We conclude that the spin injection for this system is possible only if the interface disorder is not too large.

OPTICAL AND MAGNETO-OPTICAL STUDIES OF Co/Cr MULTILAYERS

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The optical and magneto-optical (MO) properties of the Co/Cr multilayers (MLS) have been studied experimentally by spectroscopic ellipsometry and magneto-optical Kerr effect over the spectral range 0.8-5.8 eV and compared with the results of *ab initio* calculations performed with the use of LMTO method. From the hysteresis loops measured in both the polar and longitudinal Kerr geometry it was inferred that for all the Co/Cr MLS, prepared with constant Co sublayer thickness equal to 2 nm and the Cr thickness changing in the range of 0.4-3 nm, the magnetization lies in the sample plane. The MLS structures studied were modeled using supercell approach including both the perfect and diffused Co/Cr interface region. The influence of the Cr-sublayer thickness and the interface spatial extent on the optical and MO response of the MLS was investigated. Considerable reduction of the Co magnetic moment due to the substitutional disorder at the interfaces was found and strong sensitivity of the magnetic structure spatial profiles on the interface thickness and composition has been observed. It was found that the interface imperfectness is a main factor that affects both the shape and amplitude of the MO

spectra. Excellent agreement between the theoretical and experimental optical and MO spectra has been obtained.

DETERMINATION OF THE INTERFACIAL MAGNETO-OPTICAL PROPERTIES IN SPUTTERED Fe/Au MULTILAYER STRUCTURES

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The Fe/Au multilayers (MLS) prepared by dc- sputtering on GaAs(001) and Si(100) substrates with 60 nm Au buffer layer have been studied by spectroscopic ellipsometry and Kerr effects in polar and longitudinal geometry at the photon energies ranging from 0.8 to 5.8 eV. From the x-ray diffraction analysis it follows that the Fe/Au films studied exhibit well defined layered structure with the fcc crystal structure and pronounced (111) texture. The effective dielectric tensor components of the fcc Fe/Au MLS structures were derived from the experimental ellipsometry and magneto-optical (MO) spectra. In order to obtain a quantitative understanding of the MO response of the Fe/Au MLS we have performed extended multiple reflection calculations as well as calculations based on the band structure LMTO calculations for various models of the MLS structure. The results obtained show a crucial role of the interface volume and its structure in the formation of the MO response of the Fe/Au MLS. The differences between the MO properties measured for in-plane and out-of plane sample magnetization direction, firstly observed in (001) Fe/Au superlattices, are established for sputter deposited (111) Fe/Au studied and its relation with interface structure has been examined.

ATOMIC DISORDER IN SOME HEUSLER ALLOYS

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We report the influence of the local atomic disorder on the magnetic properties and electronic structure of $Ni_2(Mn_xTi_{1-x})Sn$, $Fe_{2-x}Ni_xTiSn$, $Fe_{2-x}Co_xTiSn$ and Fe_xTiSn Heusler type alloys. The electronic and magnetic properties are calculated by the spin–polarised TB LMTO method in the atomic sphere approximation (ASA) within the local–spin density approximation (LSDA). The substitution of Fe atoms onto titanium or tin positions leads to an increase of the magnetic moment. Fe_2TiSn is a nonmagnetic material whereas for the disorder alloy the magnetic ground state is obtained, in agreement with observation. The theoretical lattice parameter estimated from the minimum of the total energy for $x \geq 1.5$ was very similar to that obtained experimentally by X–ray diffraction on the Fe_xTiSn samples. In $Ni_2(Mn_xTi_{1-x})Sn$ alloy we found the critical concentration x for which the system was magnetic.

THE ELECTRICAL CONDUCTIVITY IN THE OFF-STOICHIOMETRIC HEUSLER Fe_2VX (X=Al, Ga)

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The Fe_2VX (X=Al, Ga) Heusler compounds exhibit several properties uncommon among the 3d-transition metal intermetallic compounds. The most intriguing is the semiconductor-like behavior of the electrical resistivity with simultaneous anomalously large value of electronic specific coefficient γ. The calculated electronic structure of the Fe_2VAl characterizes a deep, 0.5 eV wide, pseudo-gap centered at Fermi level (ε_F). Our recent electronic structure calculations of the off-stoichiometric $Fe_{(2+y)}V_{(1-y)}X$ ($y = \pm 0.06$) compositions have proved the existence of the narrow band located just at ε_F. In the non-magnetic state of the $y > 0$ composition the band appeared to be the almost fully occupied upper Hubbard band of the d-e_g states of the impurity Fe atoms. The presence of the band explains the large value of the γ coefficient. It may also response for the negative value of the temperature coefficient of the DC-resistivity. To investigate this we considered the two-band model of the strongly correlated narrow band coupled by the hybridization interaction with the quasi-free electron band. The model was solved by the CPA approach within the Alloy Analogy approximation and the Kubo-Greenwood formula for the DC-conductivity was applied. The calculated temperature dependence of the DC-resistivity qualitatively agree with the measured one.

HYPERFINE PARAMETERS OF THE HEUSLER TYPE $Fe_{2+x}V_{1-x}$ ALLOYS

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The hyperfine parameters (isomer shift and hyperfine magnetic field) for ^{57}Fe nucleus in the Heulser-type $Fe_{2+x}V_{1-x}$ ($x \geq 0$) alloys were calculated by means of the *ab initio* electronic structure calculation methods. The calculations performed for these alloys have shown that the Fe anti-site (AS) atoms (Fe at V positions of the Heulser Fe_2VAl) characterizes the stable (independent on concentration x) magnetic moment of magnitude of 2.2—2.5 μ_B. On the other hand the Mössbauer experimental investigations of the $Fe_{2+x}V_{1-x}$ ($x \geq 0$) alloys have indicated the presence of Fe atoms with intermediate value of hyperfine magnetic field (~15 T). The experimental data interpreted within the simple model of linear scaling (HF$\sim \mu_{Fe}$) have predicted the presence of the Fe atoms with the medium sized magnetic moment (~1.5 μ_B) which number varies with temperature and concentration. The results of calculations for the hyperfine magnetic field (HF) have explained the experimental data in the following way. The calculated magnitude of HF on Fe-AS atoms depends sensitively on the magnetization of the nearest neighborhs. The transferred part of the HF, usually small as compared the local part, reaches relatively large values and points toward opposite direction compared the local HF. The both parts of HF (local and transferred) reduce each other on Fe-AS atoms leading to the medium sized magnitude of HF despite the high value of magnetic moment of these atoms.

MAGNETIC AND HYPERFINE PROPERTIES OF ORDERED AND DISORDERED Fe-Al ALLOYS

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The magnetic moment (μ), hyperfine field (B_{hf}) and isomer shift (IS) of the Fe atoms in bcc Fe-Al alloys were calculated from first principle. The super-cell including 16 atoms (8xB2 formula unit) was constructed and several possible environments of Al atoms around iron sites in the alloy have been considered in order to study magnetic and hyperfine properties. Different contributions to hyperfine field and isomer shift were calculated separately. The variation of the μ, B_{hf} and IS at iron atoms due to presence of aluminum nearest and next-nearest neighbors was analyzed. The effect of the lattice parameter variation on the above mentioned quantities was also investigated. With increasing pressure the transition from the parallel to anti-parallel alignment of Fe-magnetic moments was found for Al concentration of 30 at.%. The transferred hyperfine field, resulted from the spin-polarization of outer 4s electrons by surrounding magnetic moments, exhibit significant dependence on the number of Al atoms in the first and the second coordination sphere of an Fe atom. The average $< \mu >$, $< B_{hf} >$ and $< IS >$ was calculated for disordered and ordered Fe-Al alloys with B2 and DO_3 superstructure by Monte Carlo simulation method. The very good agreement with experiments was found.

THE ELECTRONIC AND ELECTROCHEMICAL PROPERTIES OF THE $LaNi_5$-BASED ALLOYS

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The battery electrode materials $La(Ni - Mn - Co - Al)_5$ are substitutional derivatives of $LaNi_5$ in which La occupies site 1(a), and Ni, Mn, Al, and Co sites 2(c) and 3(g) of space group $P6/mmm$. Nanocrystalline $LaNi_5$-type materials have been prepared by mechanical alloying followed by annealing. The amorphous phase forms directly from the starting mixture of the elements, without other phase formation. The as-milled powders were heat treated at $1000K$ for 0.5h under high purity argon to form the hexagonal $CaCu_5$-type phase. The powders were examined by XRD analysis, with Co K_α radiation, at the various stages during milling prior to and after annealing. The electrochemical properties of these materials have been investigated and discharge capacity enhancement has been observed. The electronic structure has been studied by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation (*TB LMTO ASA*). The startting $LaNi_5$ is not magnetic but Al, Co, and Mn change band structure and in doped materials magnetic order is observed. The values of magnetic moments located on Mn atoms reach at leat $3\mu_B/atom$.

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THE ELECTRONIC AND ELECTROCHEMICAL PROPERTIES OF THE $TiFe$-BASED ALLOYS

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The titanium compounds TiX ($X = Fe, Co, Ni$), with $CsCl$-type structure are promissing hydrogen storage materials. The capacity of the hydrogen absorption in these compounds is known to be smaller than the value which would be expected from the crystal geometry. The high-energy milling technique is generally used to modify the surface structure and texture of materials in order to improve their physical or chemical properties. In this work we present results for $TiFe_{1-x}Ni_x$ compounds. The electrochemical properties of these materials have been investigated and discharge capacity enhancement has been observed. With increasing nickel content in $TiFe_{1-x}Ni_x$, the material showed an increase in discharge capacity which passed through a maximum for $x = 3/4$. The electronic structure has been studied by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation (*TB LMTO ASA*). A systematic study of electronic structure for $TiFe_{1-x}Ni_x$ alloys will be presented in whole range of concentration from $TiFe$ to $TiNi$ with a step of $\Delta x = 1/8$. The calculations show a coincidence between discharge capacity and calculated characteristics like charge transfer between ions and density of electronic states at the Fermi level.

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ELECTRONIC STRUCTURE AND MAGNETISM OF $\mathbf{GdTi_{1-x}Mn_xGe}$.

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RTX germanides like GdTiGe and $GdTi_{1-x}Mn_xGe$ have particularly interesting magnetic and crystallographic properties. For GdTiGe various types of crystal structure and magnetic ordering have been reported. We have found that polycrystalline compounds $GdTi_{1-x}Mn_xGe$ crystallize in the tetragonal CeScSi type of structure (I4/mmm) for $x \leq 0.7$. The crystal structure has been refind using the Rietveld method. The temperature dependence of magnetic susceptibility and electrical resistivity have been measured for $GdTi_{1-x}Mn_xGe$. GdTiGe exhibits ferromagnetic ordering at 374 K. It is noteworthy that the temperature of the transistion is very high for a rare-earth compound with non-magnetic metals. The electronic structure of the series of compounds has been investigated with use of photoelectron spectroscopy (XPS and UPS). The electronic structure of GdTiGe determined from the photoemission spectra has been found to be in good agreement with the calculations performed with the TB-LMTO method. The calculations indicate to the polarization of the *d*-bands as a main source of the high magnetic ordering temperature, due to the indirect exchange via the *d*-band. Substitution of Ti by Mn does not lead to the substantial crystallographic changes. The electronic structure and temperature of magnetic ordering also show relatively small variation with increasing Mn content.

ON THE MAGNETIC BEHAVIOUR OF $GdCo_{2-x}Cu_x$ COMPOUNDS

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The $GdCo_{2-x}Cu_x$ compounds crystallize in a cubic C15 type structure for $x \leq 0.4$. Magnetic measurements were performed in the temperature range 4.2-900 K and external fields up to 9 T. Band structure calculations were carried out by using the ab initio tight binding linear muffin tin orbitals method in the atomic sphere approximation.The compounds are ferrimagnetically ordered. The mean cobalt magnetic moments determined at 4.2 K are little dependent on composition. The saturation moments per formula unit, at 4.2 K, are in rather good agreement with those obtained from band structure calculations. The Gd 5d band polarizations were analyzed. The contribution from 4f-5d, $M_{5d}(f)$, local exchange and 5d-3d short range exchange interactions, $M_{5d}(0)$, were determined. The $M_{5d}(0)$ values are proportional to cobalt magnetizations. The paramagnetic behaviour was also analyzed. Finally, the exchange interactions were discussed in correlation with band structure calculations.

ELECTRONIC STRUCTURE OF THE RPdSb (R=Pr, Nd) COMPOUNDS

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Electronic structure of the ternary RPdSb (R=Pr, Nd) compounds was studied by the X-ray photoelectron spectroscopy (XPS). Core-levels and valence bands were investigated. The XPS valence bands are compared with the ones calculated using the spin-polarized tight-binding linear muffin-tin orbital (TB LMTO) method. The obtained results show that the valence bands are determined mainly by the Pd 4d band. The calculation of the total energy for two models of the crystal structure: an ordered of the LiGaGe-type and a disordered one of the $CaIn_2$-type indicates that in the RPdSb (R=Pr, Nd) compounds the LiGaGe-type of structure is stable. The spin-orbit splitting values determined from the XPS spectra of Pr and Nd $3d_{5/2}$ and $3d_{3/2}$ are equal to 20.6 eV for PrPdSb and 23.0 eV for NdPdSb. The analysis of these spectra on the basis of the Gunnarsson-Schönhammer model gives information on the hybridization of 4f orbitals with the conduction band, which is large for PrPdSb. Calculated value of the Pr magnetic moment is smaller than that of the free Pr^{3+} ion value, whereas the Nd magnetic moment is equal to the free Nd^{3+} ion value.

ELECTRONIC STRUCTURE OF Ce_2TSi_3 (T=Rh, Pd) COMPOUNDS

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Electronic structure of the ternary Ce_2TSi_3 (T=Rh, Pd) compounds wich crystalize in the hexagonal AlB_2 structure was studied by X-ray photoelectron spectroscopy (XPS). Core-levels and valence bands were investigated. The XPS valence bands are compared with the ones calculated using TB LMTO method. The photoemission measurements were performed using a commercial LHS 10 SPECS spectrometer with the following radiation sources:

non-monochromatized MgK_α (hν=1253.6 eV), monochromatized and non-monochromatized AlK_α (hν=1486.6 eV). The measurements were made at room temperature in high vacuum ($2 \cdot 10^{-9}$ mbar). The VB XPS spectra of Ce_2RhSi_3 and Ce_2PdSi_3 are established mainly by 4d states of Rh and Pd- atoms. The XPS spectra of 3d Ce consists of three peaks that correspond to the f^0, f^1 and f^2 configurations. The gap between energies of the f^1 states corresponding to the energy levels of $3d_{5/2}$ and $3d_{3/2}$ states give a spin-orbit splitting Δ_{SO}, which is equal to 18.7 eV for Ce_2PdSi_3 and 18.5 eV for Ce_2RhSi_3. Based on the Gunnarsson-Schönhammer theoretical model, the intensity ratio $f^0/(f^0 + f^1 + f^2)$ gives the f-occupation probability in the final state. The obtained results suggest that about 0.25 ions have the f^0 configuration. The shift of the shake down satellites in relation to the main peak is about 3.3 eV in Ce_2PdSi_3 and 3.6 eV in Ce_2RhSi_3. The intensity ratios $r = f^2/(f^1 + f^2)$ for Ce_2PdSi_3 and Ce_2RhSi_3 are near 0.5. Such r values correspond to a very large value of Δ(about 300 meV). Similar, large Δ's (about 220 eV) are observed in Ce stannides and antimonides of the 1:2:2 type.

ELECTRONIC STRUCTURE OF $Ce_2Co_{1-x}Au_xSi_3$ $(0 \leq x \leq 1.0)$ COMPOUNDS

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Properties and parameters of the electronic structure of $Ce_2Co_{1-x}Au_xSi_3$ $(0 \leq x \leq 1.0)$ compounds are presented. These compounds crystallize in a hexagonal crystal structure derived from the AlB_2-type. Macroscopic measurements suggest the change of the properties from strong Kondo regime for $x = 0$ to magnetic ordering for $x \geq 0.4$. To explain such properties of these compounds X-ray photoelectron spectroscopy (XPS) measurements were performed using a commercial LHS 10 Leybold spectrometer with non-monochromatized MgK_α ($h\nu$=1253.6 eV) radiation. The measurements were carried out at room temperature in high vacuum (10^{-9} mbar). The XPS valence bands of all the investigated compounds are formed mainly by the $3d$ Co and $5d$ Au states that was confirmed by electronic structure calculations using the ab initio self consistent tight-binding linear muffing-tin orbital (TB LMTO) method. The 4f band of Ce is well above the Fermi level and does not change with changing Au content. For both compounds the contributions of the three final states $4f^0$, $4f^1$ and $4f^2$ are observed in the Ce 3d XPS spectra. The spin-orbit splitting Δ_{SO} equal 18.7 eV for x=0.4 and 18.3 eV for x=0.6, 0.8 and 1.0. Based on the Gunnarsson-Schönhammer theoretical model the hybridization energy Δ is determined. The obtained results suggest that the hybridization energy Δ changes from 28 meV, for x=0.4 to 62 meV for x=1.0

ELECTRONIC STRUCTURE OF CUBIC $DyCu_5$

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Binary RCu_5 (R=heavy rare earth) compounds can crystallize in two different allotropic structures: (i) low-temperature cubic and (ii) high-temperature hexagonal forms.

We report on the electronic properties of Dy-Cu compound in cubic $AuBe_5$-type structure. The single phase sample was produced in Ar atmosphere using conventional one wheel melt-spinning equipment as long ribbon.

The valence band spectra of the compound were investigated by X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS). Results of ab initio calculation of the electronic structure using the tight-binding linear muffin-tin orbital (TB LMTO) method are compared with experimental data.

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PROJECTED DENSITY OF STATES AND MOMENTS IN TRANSITION METALS WITH SPIN DENSITY WAVES

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Most calculations involving the Kohn-Sham (KS) equations such as *ab initio* molecular dynamics calculations [1], require a simplification of these equations. Our approach is based on the moment technique [2], which is an interpolation of electronic structure. The KS Hamiltonian of transition metal with spin density waves (SDW) is given in the form [3]. The KS equations, the projected density of states (PDOS), moments of PDOS and Anderson's atomic orbitals are self-consistently calculated. The moments contain the dependence of KS orbitals on the interatomic spacing and the SDW parameters, as given by the Hellmann-Feynman theorem. The moments enable us to analytically express the PDOS, the total electronic energy and the chemical potential as functions of the SDW parameters (SDW wave vector and polar angle of magnetic configuration). We use the adiabatic local density approximation. Calculations are confined to second moments of PDOS at atomic orbitals.

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ELECTRONIC STRUCTURES AND VARIOUS PHYSICAL PROPERTIES OF Ni_3Al ALLOY

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The magnetic, optical and magneto-optical properties of slightly off-stoichiometric γ'-phase Ni_3Al alloy ($Ni_{0.771}Al_{0.229}$) have been investigated experimentally and theoretically. The optical-conductivity spectrum exhibits a multiple-peak structure in the near-infrared region. It is shown that the fine structure of the low-energy absorption features is originated from the spin-ordering in the alloy and experimentally shown that this fine structure persists up to room temperature. This feature was theoretically predicted, but not experimentally confirmed previously. The temperature dependencies of the magnetic, optical and magneto-optical properties of $Ni_{0.771}Al_{0.229}$ alloy can be ascribed to the presence of magnetic inhomogeneity in the sample. DC magnetic-susceptibility measurements confirms the existence of magnetic inhomogeneity in the alloy. The $\chi(T)$ curve exhibits two magnetic transitions, one at 87.5 K and the other at 252K. The spin ordering and Ni enrichment, or Ni clusters, play a key role for the physical properties.

THEORETICAL SEARCH FOR MAGNETIC HALF-HEUSLER SEMICONDUCTOR

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We present electronic structure of half-Heusler $CoTi_{1-x}T_xSb$ and $FeV_{1-x}T_xSb$ with $x = 0.001, 0.005, 0.01$ and 0.05 derived from the charge and spin-selfconsistent KKR-CPA computations. Experimentally, both parent compounds were found to show semiconducting properties [1]. This was supported by the band structure calculations [2], which gives an energy gap as large as 0.95 eV (CoTiSb) and 0.46 eV (FeVSb). Among transition metal impurities doped in the aforementioned semiconductors, Cr and Mn atoms exhibit a strong polarisation of density of states, if substituting selectively on Ti- and V-site in CoTiSb and FeVSb, respectively. The calculated magnetic moment on Mn is found to be on average as large as 2.5 μ_B and 3.2 μ_B in FeVSb and CoTiSb, respectively. Inspecting total DOS near the gap in these magnetic systems we find a behavior very similar of half-metallic magnetics than of magnetic semiconductors. Moreover, if impurity concentration decreases the energy gap tends to open for both spin channels.

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EFFECT OF LOCAL ENVIRONMENT ON THE MAGNETIC PROPERTIES OF THE $(Cu_{1-x}Co_x)_2$MnSn ALLOY

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The electronic structure and the ground state properties of the quaternary Heusler alloy $(Cu_{1-x}Co_x)_2$MnSn has been studied using the self-consistent the spin-polarized tight-binding linear muffin-tin orbital (TB-LMTO) method. The self-consistent band calculations were performed for the experimental lattice constant [1]. The $(Ni_{1-x}Co_x)_2$MnSn compound has been calculated for the supercell structure and for the following values of the parameter x: 0; 0.125; 0.25; 0.375; 0.5; 0.625; 0.75; 0.875; 1.0. The supercell structure with 16 atoms in the cell can be divided into 16 simple cubic sublattices. Eight of them are occupied by Mn and Sn atoms ordered in a L21 structure, whereas Ni and Co randomly occupy the remaining eight sublattices. The magnetic properties are in good agreement with experimental data presented in [1]. In particular the observed linear change of total magnetic moment with concentration of Co is reproduced by our calculations. We present the values of local magnetic moments of the Co and Cu atoms for various possible configurations. The dependence of magnetic moments on the local environment is studied for all concentrations.

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MAGNETISM AND BAND STRUCTURE OF Co/Ti MULTILAYERS BY AB-INITIO METHODS

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We present the electronic structure and magnetism of Co–Ti systems, in which Co and Ti atoms are distributed in the planes of the different crystallographic structures (bcc, hcp and $L2_1$). The band structure and magnetic moments are calculated by the spin–polarised TB LMTO, ASW, and FP LAPW methods within the local spin density approximation. The number of Co and Ti layers changes from 1 to 10 depending on the type of structure. We study also the effect of alloying between Co and Ti layers. The value of the magnetic moment of Co depends strongly on the local environment. We observe that the value of magnetic moment of Co decreases almost two times when the Co is surrounded by Ti atoms.

LOCAL MAGNETIC MOMENTS IN $Fe_{3-x}Cr_xSi$ AND $Fe_{3-x}Cr_xAl$ ALLOYS

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We present the results of self-consistent spin-polarised TB-LMTO band structure calculations of Fe_3Si and Fe_3Al substituted by chromium. The ordered alloys have DO_3-type crystal structure with two sites of iron that are not equivalent. The aim of the paper is to show an influence of the local environment on the distribution of hyperfine magnetic fields. All the nearest neighbour atomic configurations corresponding to the observed sextets contributing to the Mőssbauer spectra are analysed. Comparing the total energies of the completely ordered systems with the energies of the configurations with partial disorder between iron and silicon or iron and aluminium sublattices we conclude that the ordering tendency in Fe_3Si is stronger than in Fe_3Al alloy.

NONCOLLINEAR MAGNETISM ON UFe_xAl_{12-x} SERIES: AB-INITIO CALCULATIONS

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The UFe_xAl_{12-x} series has been the object of a systematic experimental study in single crystals with different compositions [1]. Several measurements technics were used in Ref. [1] to suggest a magnetic phase diagram of the system. Three different ranges of composition were found to have different magnetic behavior: $x < 4 + \delta_1$, $4 + \delta_1 < x < 5 - \delta_2$, and $x > 5 - \delta_2$. The UFe_4Al_8 and UFe_5Al_7 compounds belong to two different regions of the phase diagram. DFT calculations and symmetry analysis for these two compounds [2, 3] contributed to the understanding of the origin of the complex magnetic behavior of the series. In order to complete the systematic study of the series we report calculations of the magnetic properties of $UFe_{4.5}Al_{7.5}$. The latter compound belongs to the third and the most interesting region of the phase diagram with two magnetic phase transitions. The symmetry analysis determines a magnetic structure with two noncollinear sublattices which is different from that proposed in Ref. [1] This is confirmed by the calculations which yield a magnetic moment in fair agreement with experimental data. We also discuss the phase diagram of the series based on both the experimental and the ab-initio studies.

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PROPERTIES OF THE UFe_5Sn COMPOUND: ELECTRONIC STRUCTURE AND X-RAY PHOTOEMISSION

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Recently synthesized compound of the composition UFe_5Sn crystallizes in the orthorhombic $CeCu_5Au-$type structure having $Pnma$ space group [1]. The unit cell has complex structure, 28 atoms in the unit cell: the iron atoms occupy four inequivalent sites, and uranium and tin occupy one type of site, each. The distance between uranium atoms, equal to 4.89 Å, is well above Hill limit (~ 3.4 Å) and suggests the possibility of an appreciable uranium magnetic moment. Also magnetic moments located on the iron atoms should be distinct because of different local environments for inequivalent sites. The electronic structure has been studied by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation (TB $LMTO$ ASA). The iron magnetic moments are antiparallely oriented to the uranium moments. The photoemission spectra, calculated from densities of electronic states, are compared with experimental ones [2].

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ELECTRONIC STRUCTURE OF THE URANIUM MONOSTANNIDE USn

A. Szajek

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The uranium monostannide USn crystallizes in the orthorhombic $ThIn$-type structure with the space group $Pbcm$ [1]. Uranium and tin atoms each occupy three crystallographic positions. The uranium atoms located in (4c) sites form metallic chains running along c axis, with a $U-U$ interatomic distance of 3.10 Å. USn orders ferromagnetically below $T_C = 55K$, with an ordered moment of $1.20\mu_B/U$ measured on a polycrystallized sample. Because of short distance $U(4c)-U(4c)$ and expected hybridization with the conduction-band electron states it would be interesting to know if this uranium sublattice is also ordered magnetically. $Ab-initio$ calculations would clarify this situation. In this work, spin-polarized band structure calculations results will be presented based on the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation (TB $LMTO$ ASA). The calculations showed that all three types of uranium atoms are magnetically ordered and their moments depend on local environments.

Work supported by the KBN Grant No. 2 P03B 023 22

[1] P. Boulet and H. Noël, *Solid State Commun.* **107** (1998) 135

SEMICONDUCTING PROPERTIES OF DISORDERED HALF-HEUSLER SYSTEMS

J. Toboła[a], G. Venturini [b] and S. Kaprzyk[a]

[a]*Fac. of Phys. and Nucl. Techniques, Univ. of Mining and Metall.,*
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Recently, a composition induced metal-semiconductor-metal crossover has been detected in the $\mathrm{Fe}_{1-x}\mathrm{Ni}_x\mathrm{TiSb}$ half-Heusler system using resistivity and thermopower measurements and supported by electronic structure computations based on the KKR-CPA method [1]. Such an unusual behavior is also expected in other disordered half-Heusler phases possessing the critical number of the valence electrons. We present results of electronic structure calculations on $\mathrm{Fe}_{1-x}\mathrm{Pt}_x\mathrm{ZrSb}$, $\mathrm{Ru}_{1-x}\mathrm{Ni}_x\mathrm{ZrSb}$ and $\mathrm{Ru}_{1-x}\mathrm{Pd}_x\mathrm{ZrSb}$ which are isoelectronic to the aforementioned system. The onset of semiconducting state, when alloying parent compounds (metals), is detected through a remarkable modification of density of states as a function of composition. Moreover, a shift of the Fermi level (E_F) from valence to conduction states for $x \approx 0.5$, should have an apparent effect on conductivity and thermopower behavior. The appearance of the energy gap at E_F in the disordered alloys is also in line with previous studies on ordered half-Heusler systems, which revealed a high propensity for forming bandgaps in the compounds having 18 valence electrons. [1] J. Toboła et al., Phys. Rev. **B** 64, 155103 (2001).

LIST OF PARTICIPANTS

invited speakers and participants who used *ab–initio* methods in their presentations;

full list of participants, including addresses, is available on the PM'02 WWW page:

http://www.ifmpan.poznan.pl/zp2/pm02.html

Bogdan Andraka, Department of Physics, University of Florida, GAINESVILLE, USA
Klaus Baberschke, Institut für Experimentlphysik, Freie Universität Berlin,
BERLIN, GERMANY
Józef Barnaś, Department of Physics, A. Mickiewicz University, POZNAN, POLAND
and Inst. of Molecular Physics, Polish Acad. of Sciences, POZNAŃ, POLAND
Gunnar Borstel, Dept. of Physics, Univ. of Osnabrück, OSNABRÜCK, GERMANY
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S.C. Erwin, Naval Research Laboratory, WASHINGTON DC, USA
J.E. Frackowiak, Inst. of Phys. and Chem. of Metals, Univ. of Silesia, KATOWICE, POLAND
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Andrzej Szytuła, Institute of Physics, Jagiellonian University, KRAKÓW, POLAND
W. Temmerman, Daresbury Laboratory, DARESBURY, WARRINGTON, U.K.
R. Tetean, Faculty of Physics, Babes-Bolyai University, CLUJ-NAPOCA, ROMANIA
Janusz Toboła, Faculty of Physics and Nuclear Techniques, Academy of Mining and Metallurgy, KRAKÓW, POLAND
Ilja Turek, Inst. of Physics of Materials, Czech Acad. of Sciences, BRNO, CZECH REPUBLIC
Stanisław Uba, Inst. of Exp. Physics, University of Białystok, BIAŁYSTOK, POLAND
Luba Uba, Inst. of Exp. Physics, University of Białystok, BIAŁYSTOK, POLAND
P. Wachter, Laboratorium fuer Festkörperphysik, ETH , ZÜRICH, SWITZERLAND
E. Wawrzyńska, Inst. of Physics, Jagiellonian University, KRAKÓW, POLAND

P.E. Wigen, Department of Physics, Ohio State University, COLUMBUS, USA
Adriana Wrona, A. Chełkowski Inst. of Physics, Silesian Univ., KATOWICE, POLAND
Karol I. Wysokiński, Inst. of Physics, M. Curie Skłodowska University, LUBLIN, POLAND
Jan Zaanen, Lorentz Inst. for Theoretical Physics, Leiden University,
LEIDEN, THE NETHERLANDS
Maciej Zwierzycki, Univ. of Twente, Faculteit der Technische Natuurkunde/CMS,
ENSCHEDE, THE NETHERLANDS

6 General Workshop/Conference Announcements

6.1 IWOSMA2 Workshop

Second Announcement

2nd International Workshop on Orbital And Spin Magnetism of Actinides (IWOSMA2)

Chair: J.G. Tobin, LLNL

Co-Chair: D.K. Shuh, LBNL

Web-site: http://www.iwosma.org

The second IWOSMA meeting will be held on October 13-15, 2002, at the Claremont Resort and Spa in Berkeley, CA, USA. A welcoming reception and meeting initiation will be held on the evening of Sunday, October 13. Oral and poster sessions will continue throughout Monday, October 14 and Tuesday, October 15. A workshop banquet is being planned for the evening of Monday, October 14. A partial list of invited speakers is shown below. Although many of the presentations will be invited talks, abstracts for contributed talks and posters will be solicited in the near future. Details of abstract submission, as well as meeting registration and lodging reservations, will be available from the meeting web-site (iwosma.org) in the near future.

Further related information can be gotten from the following web-sites.

First IWOSMA Meeting:

`http://srs.dl.ac.uk/msg/MSG_Events_IWOSMA.html`

ALS Users Meeting (October 10-12):

http://www-als.lbl.gov/als/usermtg/

SSRL Users Meeting (Oct 7-9):

http://www-ssrl.slac.stanford.edu/conferences/ssrl29/Claremont

Resort and Spa: http://www.claremontresort.com/

Partial List of Invited Speakers

N. Edelstein, LBNL, USA
G. Lander, Karlsruhe Facility, Germany
B. Sadigh, LLNL- Chemistry, USA
P. Soderlind, LLNL- Physics, USA
G. van der Laan, Daresbury Laboratory, United Kingdom

6.2 EPENS'02 Workshop Announcement

International Workshop on Electron-Phonon Effects in Nanosystems (EPENS'02)

September 23-25, 2002, Montauk NY

In "Gordon Conference" style, this workshop will be chemistry and physics equally, aiming to shine light on previously unexplored connections between vibronic effects in molecular behavior and electronic properties of nanosystems.

Details are on the conference web page

`http://felix.physics.sunysb.edu/~vibronic/`.

The Montauk Yacht Club Hotel has 107 rooms on the water, a very good kitchen, and pleasant meeting space. Montauk is on the very eastern tip of Long Island. It is a resort area famous for fishing, whale or bird watching, swimming, sailing, etc. Slightly to the west, the Hamptons are famous for a number of other things, some of which have cooled down by September. This allows us a very reasonable rate at the Hotel.

Please join us for a great meeting. Come early for the reception at 4pm on Sunday September 22.

Yours truly,

The Organizing Committee

(Philip B. Allen, Marshall Newton, Laszlo Mihaly, Vasili Perebeinos)

7 General Job Announcements

Postdoctoral Position

COMPUTATIONAL MATERIALS SCIENCE - MIT

A postdoctoral research position is available jointly in the groups of Professors Ceder and Marzari, in the Department of Materials Science and Engineering of the Massachusetts Institute of Technology.

The research will cover the application of electronic-structure approaches to predict the structural/electronic/optical properties of nanosystems, in a multi-disciplinary environment and in close collaboration with different experimental groups.

The position is initially for one year, renewable to a second. Expertise in electronic-structure approaches is required, and a materials-oriented background highly desirable.

Interested candidates should e-mail a curriculum vitae (publication list and names and contact informations for two/three references) to

gceder@mit.edu and marzari@mit.edu

(PostScript or PDF are preferred), or via regular mail to

Kristin Gunst
Ceder/Marzari Postdoc
Department of Materials Science and Engineering
13-5062 Massachusetts Institute of Technology
77 Massachusetts Avenue
Cambridge MA 02139-4307
USA

Consideration of candidates will begin immediately and will continue until the position is filled.

June 19, 2002 — http://nnn.mit.edu/postdoc

Postdoctoral Position

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

A postdoctoral position tenable for up to two years is immediately available at the Theory Department of the Fritz-Haber-Institut in Berlin-Dahlem, which is headed by Prof. Matthias Scheffler. The research project focuses on the *ab initio* investigation of the electronic and optical properties of surfaces. Both semiconductors and transition-metal compounds that play an important role as catalysts will be studied. The main goal is to understand how surface reconstruction, defects and adsorbates influence the properties of these materials in technological applications. In order to describe quasiparticle band structures and excitation spectra accurately, advanced Green function schemes such as the GW approximation for the electronic self-energy are employed. Applicants for this position should have a strong background in electronic-structure calculations. Experience with excited-state methods is desirable but not a requirement.

The postdoctoral position is funded through the Research Training Network "Nanoscale Photon Absorption and Spectroscopy with Electrons" (NANOPHASE). To be eligible for an appointment under the network contract candidates must be (i) aged 35 years or less, (ii) a citizen of a member state of the European Union or an associated state of the Fifth Framework Programme, excluding Germany, or have resided within the European Union for at least five years prior to the appointment, (iii) resident and working in Germany for less than 12 months within the last two years.

Interested candidates should send a curriculum vitae, highlighting their main achievements and experience, together with a publication list to the address given below. Electronic applications are welcome, and reference letters will be given proper consideration. Please feel free to send an e-mail for informal inquiries. Applications are accepted until the position is filled.

Dr. Arno Schindlmayr
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4–6, 14195 Berlin, Germany
E-mail: schindlmayr@fhi-berlin.mpg.de

Further information about the group can be found at

http://www.fhi-berlin.mpg.de/th/th.html.

Postdoctoral Position - First-Principles Calculations

Multiscale Materials Modeling Program

Ford Motor Company / Penn. State University

A new postdoctoral research position is open for an exciting new multidisciplinary program involving multiscale materials modeling. The program involves a team of investigators at the Ford Research Laboratory, Penn St. University, and the National Institute of Standards and Technology (NIST). The postdoctoral research associate should have specific experience with first-principles methods and computational materials science. The associate will strongly interact with our team, consisting of a broad range of scientists with expertise in the modeling areas of first-principles (Dr. C. Wolverton, Ford), computational thermodynamics (Prof. Z.-K. Liu, Penn St.), phase-field microstructural modeling (Prof. L.-Q. Chen, Penn St.), and finite element property prediction (Dr. S. Langer, NIST), as well as computer scientists and mathematicians. The program will be focused on technologically important multicomponent Al alloy systems. Although the official hire will be at Penn State, the researcher will have the opportunity to spend an extended period of time at the Ford Research Laboratory in Dearborn, Michigan. Initial appointment will be for one year, and may be renewed annually, upon mutual agreement. To apply, please send a copy of your resume and names of three references to:

Dr. Chris Wolverton
Ford Motor Company
MD3028/SRL, P. O. Box 2053
Dearborn, Michigan 48121-2053
cwolvert@ford.com

Clarifications or further details can be obtained via e-mail to *cwolvert@ford.com.*
Penn State University is an equal opportunity employer.

Nanoelectronics at the Quantum Edge
Postdoctoral Research Assistant in Modelling of Carbon Nanostructures
Research Staff Grade RAIA / Salary: 17,626 - 26,491 GBP
Job Ref: DJ02/029

Oxford and Cambridge Universities are working together with Hitachi Europe Ltd. to produce radically new devices for future computing, in a project jointly funded by a Foresight LINK Award from the Department of Trade and Industry and Hitachi Europe Ltd. The project brings together research in physics, chemistry, materials science and electronics engineering to make prototype structures for advance conventional computing and for the new field of quantum computing. See www.nanotech.org. Applications are invited for a postdoctoral position in the first-principles modelling of the atomic and electronic properties of endohedral fullerenes within single walled carbon nanotubes. This position is funded until 30 September 2004 and will be supervised by Professor David Pettifor FRS.

The successful applicant will be expected to interact closely with experimentalists performing HREM, STM, EELS and Raman characterization within this LINK programme. Candidates should have a good first degree and completed a doctorate (by the time of appointment) in physics, chemistry or materials, and should show evidence of the required first principles modelling skills. Excellent verbal and written communication skills in English, and the ability to work independently and in a team within an agreed time-scale are essential.

Before submitting an application, candidates should obtain further particulars available from The Deputy Administrator (Teaching), Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH (email: posts@materials.ox.ac.uk), or telephone 01865 273750 quoting reference: DJ02/029. The closing date for applications is 02 August 2002 and interviews are currently planned for the 29 August 2002. Further information on the Department may be found on the web-site: http://www.materials.ox.ac.uk

Postdoctoral Research Assistant
Modelling Phase-Change Materials
Research Staff grade RAIA / Salary: 17,626 - 26,491 GBP
Job Ref: DJ02/033

Applications are invited for a postdoctoral position, available for up to three years, to model electron transport in phase-change materials. The project is funded by the Hewlett-Packard Laboratory (HPL) in Palo Alto as part of ongoing research into advanced data storage devices. The research will involve the extension of a highly-successful Monte Carlo model for film growth to ternary systems and the development of an in-house Tight-Binding code for electron transport to phase-change materials of interest to HPL. The research programme will be led by Professor David Pettifor FRS.

The successful applicant will be expected to interact closely with experimentalists at HPL, visiting Palo Alto at least every six months. Candidates should have a good first degree and completed a doctorate (by the time of appointment) in physics, materials or a related physical science subject, and should show evidence of the required modelling skills, together with knowledge of their fundamental concepts. Excellent verbal and written communication skills in English (the project language), and the ability to work to agreed time-scales, both independently and in a team, are essential.

Before submitting an application, candidates should obtain further particulars available from The Deputy Administrator (Teaching), Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH (email: posts@materials.ox.ac.uk), or telephone 01865 273750 quoting reference: DJ02/033. The closing date for applications is 9 August 2002 and interviews are planned for 30 August 2002. Further information on the Department may be found on the web-site: http://www.materials.ox.ac.uk

Two postdoctoral positions in Condensed Matter Theory

Center for Materials Research and Analysis
Department of Physics and Astronomy
University of Nebraska-Lincoln
Lincoln, NE 68588-0111

Applications are invited for two postdoctoral positions to conduct research in theory of electronic, magnetic and transport properties of magneto-electronic nanostructures. The successful candidates will join the theoretical group of Professors Jaswal and Tsymbal working in a close collaboration with experimental groups studying advanced electronic, ferromagnetic and ferroelectric materials.

Required qualifications: PhD in Physics or a closely related field with strong research accomplishments in condensed matter/materials science theory, expertise in electronic band structure calculations and/or micromagnetic modeling; the ability and interest to pursue challenging interdisciplinary problems; and good communication skills.

The appointments are initially for one year, with the possibility of renewal up to four years. Salary is commensurate with qualifications and experience. Review of applications will begin immediately and will continue until suitable candidates are found. Applicants should send curriculum vitae, list of publications, description of research interests and names, phone numbers, and e-mail addresses of three references.

Contact:

Evgeny Y. Tsymbal
Associate Professor in Physics
University of Nebraska-Lincoln
Department of Physics and Astronomy
159 Behlen Lab
Lincoln, NE 68588-0111
phone: (402) 472 2586
fax: (402) 472 2879
e-mail: tsymbal@unl.edu

COMPUTATIONAL SCIENTIST

National Renewable Energy Laboratory (NREL) in Golden, Colorado

The National Renewable Energy Laboratory (NREL) in Golden, Colorado is the U.S. Department of Energy's premier laboratory for renewable energy and energy efficiency. Our mission is to develop renewable energy and energy efficiency technologies and practices, advance related science and engineering and transfer knowledge and innovations to address the nation's energy and environmental goals.

We are currently seeking candidates for a Computational Scientist position. As part of the new initiative in Computational Sciences, this position offers the opportunity to develop and implement innovative solutions that support and advance the Lab's mission. The successful candidate must have a strong computational physics background and demonstrated experience developing numerical methods and large parallel simulation codes. The selected individual will be expected to both collaborate with existing research groups (e.g., solid state theory, material science, chemistry) and conduct independent research. Candidates must have a PhD in physics, computer science, applied math or related technical fields (or equivalent experience) and two years of related work experience. For detailed information about this position, please visit our web site at

http://www.nrel.gov/hr/employment/jobs/html...

Our campus-style setting is located just west of Denver and south of Boulder. This location offers the conveniences of an urban setting, while the close proximity to the Rocky Mountains provides many opportunities for a variety of year-round outdoor activities.

To apply for this position, please submit your resume and cover letter by fax, e-mail or regular mail to:

Human Resources (Req E5300-952)
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401
Fax: 303/384-7570
`Email: nrel_employment@nrel.gov`

NREL is an equal opportunity employer committed to diversity.

Postdoctoral and Term Research Staff Positions
The National Research Council of Canada

The National Research Council of Canada has recently funded a large-scale computational material science proposal. This project will involve the development of codes that will allow multi-length and time scale predictions of material properties. Several positions (postdoctoral and term research staff) are available immediately. These positions are funded for up to 3 years at competitive salary scales.

The research will involve the development of efficient parallalizable scalable quantum codes and codes for classical molecular dynamics. Potential candidates should have interest and/or experience in code development as well as the development of "handshake" algorithms that will allow interfacing of the codes with atomic, molecular, nano, and macroscopic calculation of material properties.

Interested recent Ph.D recipients and post-doctoral candidates should send a copy of the CV and a brief research description to Dr. John S. Tse at John.Tse@nc.ca.

J.S. Tse
Program Leader
Theory and Computation Program
Steacie Institute for Molecular Sciences
National Research Council of Canada

Three PhD Positions: Computational Materials Science of (Semi)conducting Polymers

Universities of Eindhoven, Nijmegen and Twente, The Netherlands

In a joint project between the three universities and Philips Research three fundamental issues concerning the electronic structure of conjugated organic polymers will be studied (1) electron-phonon coupling and polarons (Eindhoven), (2) electron injection in plastic electronics (Nijmegen), and (3) metal organic interfaces (Twente). These issues are of crucial importance in the further development of plastic electronic devices such as transistors and light emitting diodes, based on these materials. We are looking for excellent candidates with a top grade M.Sc. degree in theoretical physics or chemistry and a strong interest in computational physics. Your formal employer will be the Foundation for Fundamental Research on Matter (FOM, see www.fom.nl). Enquiries and applications (including a CV, list of university grades, publications if any, as well as the names of referees) should be sent to:

(for 1)

Dr. P.A. Bobbert,
Polymer Physics, Dept. of Applied Physics, Eindhoven Univ. of Technology,
PO Box 513, NL-5600 MB Eindhoven, The Netherlands
E-mail: P.A.Bobbert@tue.nl

(for 2)

Prof.dr. R.A. de Groot,
Electronic Structure of Materials, Dept. of Science,
Mathematics and Computing Science, Univ. of Nijmegen,
PO Box 9010, NL-6500 GL Nijmegen, The Netherlands
E-mail: robdg@baserv.uci.kun.nl

(for 3)

Dr. G. Brocks,
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PO Box 217, NL-7500 AE Enschede, The Netherlands
E-mail: G.Brocks@tn.utwente.nl

A full version of this advertisement is available at:

http://www.fom.nl (click on 'Vacatures')

Further info:

http://www.phys.tue.nl/pfy/pfy.htm
http://www-tvs.sci.kun.nl/esm/index.html
http://www.tn.utwente.nl/cms

PhD Position in Computational Magnetism
Trinity College Dublin, Ireland

One PhD studentship in Computational Magnetism is available in the Computational Physics group at Trinity College Dublin. The project will involve the development and the numerical implementation of the LDA+U method within a localized basis set algorithm for density functional theory, for calculating the electronic structure of strong correlated materials. The main aim of the project is to investigate the structural, magnetic and transport properties of wide-gap diluted magnetic semiconductors such as (Ga,Mn)N and (Zn,Co)O. The project, under the supervision of Dr. S.Sanvito, will involve a strong collaboration with Prof. N.A.Hill's group at University of California Santa Barbara, and visiting periods are planned.

The studentship will commence on the 1st October 2002 with an annual salary of 11.000 Euro. The Physics Department at Trinity College has a long and distinguished history of research. Currently the department is host of the prestigious first phase of Science Foundation of Ireland Nanotechnology projects, attracting world class researchers and establishing internationally competitive facilities. Finally it is worth mentioning that Dublin is a vital, young European capital, and a very pleasant place to live.

Candidates for this studentship are invited to send a CV, and the full contact address of two referees by post or e-mail to:

Dr.Stefano Sanvito
Department of Physics
Trinity College
Dublin 2, Ireland
Tel:+353-1-6081055
Fax:+353-1-6711759
E-mail: sanvitos@tcd.ie

Information about the research activity may be found at:

http://www.tcd.ie/Physics/People/Stefano.Sanvito/

Further particulars regarding the Studentship may also be obtained from Dr.Sanvito.

Marie Curie Fellowships

Ecole Polytechnique, Palaiseau, Paris, France

Marie Curie Training Site

Several Marie Curie host fellowships for PhD students will be available at the Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau (Paris, France), in collaboration with Dr. Lucia Reining. The fellowships are for 6 to 12 months, the first one starting from October 2002. The research will be inserted in the framework of ongoing collaborations within the EU Research Training Network "NANOPHASE: Nanoscale photon absorption and spectroscopy with electrons." The overall topic of the network research is the theory of nanometer-scale structures and the spectroscopic processes that can be used to characterise those structures, their electronic and optical properties, and their growth. These are studied using fundamental theory and state-of the-art ab initio computer simulations.

(Please see also `http://www-users.york.ac.uk/~rwg3/nanophase.html`).

In particular, the group in Palaiseau has been working during the last years in the field of one - and two-particles Green's functions calculations (GW, excitons in optical absorption), and Time-Dependent Density Functional Theory. These topics should be developed further, concerning both theory and numerics, preferably towards applications to nanostructures and oxides including defects. The work will include the determination, within DFT-LDA, of structural relaxations, the calculation of the corresponding quasiparticle levels using the GW method, and absorption and luminescence spectra including local field and excitonic effects. Computer codes are already available in Palaiseau. Computational facilities include locally several Compaq DS-20 Workstations, and national supercomputer time.

Candidates should be working on a thesis subject close to these topics. He/she should have a strong background in theoretical condensed matter physics and like to perform both analytical and numerical work.

The first position is for 6 months, starting from October 1, 2002. The deadline for applying for this position is Monday, July 8. The topic is the ab initio calculation of the optical and electron energy loss spectra of semiconductor clusters, both free-standing and embedded. In particular, we will study the role of local field effects, and the effects of confinement. The calculation of the dynamical dielectric matrix will be performed as a first step within Time-Dependent Density Functional Theory. The induced exchange-correlation contribution will be evaluated in the adiabatic local density approximation (TDLDA), and by an improved scheme, taking into account long-range correlations, which has been recently developed in Palaiseau [1]. The calculation of the dielectric function will then be iterated, when appropriate, by the simultaneous solution of the Dyson and Bethe-Salpeter equations [2,3].

[1] L. Reining, V. Olevano, A. Rubio, and G. Onida, Phys. Rev. Lett. **88**, 066404 (2002).

[2] S. Albrecht, L. Reining, R. Del Sole, and G. Onida, Phys. Rev. Lett. **80**, 4510 (1998).

[3] G. Onida, L. Reining, and A. Rubio, Reviews of Modern Physics, **74**, 601 (2002).

If you are interested in this or upcoming possibilities, please don't hesitate to contact

Lucia Reining E-mail: Lucia.Reining@polytechnique.fr Tel.: +(33) (0)1 69333690 Fax: +(33) (0)1 69333022

Magnetic Spectroscopist
Daresbury Laboratory, Warrington, U.K.

A vacancy exists for a Band 4 in the Magnetic Spectroscopy Group (MSG). The job requires instrumentation skills and lab management together with a keen interest in magnetism exploring recent advances in x-ray absorption, photoemission and scattering using polarized synchrotron radiation. The possibility exists to take up either a full time position or, in case the candidate has already an existing UK academic position, a joint appointment or a secondment.

The successful applicant will have the day-to-day responsibility to run the Magnetic Spectroscopy Lab and to co-ordinate synchrotron radiation-related support activities in collaboration with users and staff. This involves a variety of beam line and off line instruments, such as a superconducting magnet, fast-switching electromagnet for x-ray magnetic circular dichroism (XMCD), high-resolution low-energy electron diffraction (HRLEED) and diffractometer for soft x-ray resonant magnetic scattering.

Magnetic Spectroscopy at Daresbury has been recognised as a main area of in-house and collaborative research. The group has a long-standing international reputation and is also involved in long-term experimental programmes at next-generation SR facilities, such as the ESRF in Grenoble and the Tesla Test Facility in Hamburg. Among the future developments pursued are x-ray magnetic holography, x-ray resonant magnetic Raman scattering and time resolved magnetic spectroscopy.

Applicants should have research experience in one or more of the following fields: scientific application of synchrotron radiation, magnetism and surface science; with a PhD, preferably in physics or similar. An important criterion for selection is the candidate's research activity as demonstrated by scientific output. It is expected that the successful candidate is able to balance lab management, user support and collaboration with a cutting-edge research career within magnetic spectroscopy. Starting salary is up to 32,380 GBP on a pay range from 25,900 to 35,620 GBP per annum according to relevant experience. An index-linked pension scheme, flexible working hours and a generous leave allowance are also offered. In case of a joint appointment the fraction of the salary proportional to the time spend at Daresbury (typically 50be expected.

Further information on this post is available from Prof G van der Laan, tel: +44 (0)1925-603448, email: `g.van_der_laan@dl.ac.uk` , web: http://srs.dl.ac.uk/msg,

Application forms can be obtained from: Recruitment Office, Human Resources, Daresbury Laboratory, Daresbury, Warrington, Cheshire, WA4 4AD. Telephone (01925) 603114, or email recruit@dl.ac.uk, quoting reference VND151/02. More information about CLRC is available from CCLRC's World Wide Web pages at http://www.cclrc.ac.uk

All applications must be returned by 20 August 2002.

The Council for the Central Laboratory of the Research Councils (CCLRC) is committed to Equal Opportunities. CCLRC is a recognised Investor in People. A no smoking policy is in operation.

8 Abstracts

Electronic and Magnetic Structure of URhGe

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Abstract

A consistent picture of the magnetic properties and electronic structure of the superconducting itinerant ferromagnet URhGe is obtained with the local spin density approximation (LSDA). The LSDA calculations reproduce both the magnitude of the observed moment, composed of strongly opposing spin and orbital parts, and the magnetocrystalline anisotropy. It is shown that the canted magnetic structure of URhGe can originate from non-collinear arrangement of U atom orbital magnetic moments, while the spin magnetic moments are ferromagnetically ordered.

(Phys. Rev. B 65 - Rapid Comm., 180509 (2002))
Manuscript available from: shick@fzu.cz

Quantum-size effects in ultrathin Ag films on V(001): Electronic structure and photoelectron spectroscopy

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Abstract

First-principles calculations are performed to investigate in detail the electronic structure of ultrathin Ag films deposited on V(001). Quantum-well states in the Ag films show the typical dispersion with film thickness, but their spectral densities differ significantly from those of model systems. *Ab-initio* calculations for several systems (bulk, surfaces, interfaces, and thin films) reveal as origins band-structure effects and hybridization between Ag and V states. Quantization effects show up as intensity oscillations in the constant-initial-state mode of photoelectron spectroscopy. Earlier experimental investigations, which reported inconsistencies with typical manifestations of quantization effects, are discussed.

(Submitted to Phys. Rev. B)
Manuscripts available from: henk@mpi-halle.de

Interaction between oxygen and single self-interstitials in silicon

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Abstract

Unlike vacancy-oxygen defects, the role of Si interstitials (I) when trapped by interstitial oxygen (O_i) is far from clear. In an attempt to enlighten the the interaction between these complexes, we report *ab-initio* modeling of $I\mathrm{O}_i$ defects. Calculated electrical levels, vibrational modes and other properties are compared with the available experimental data. We end with the assignment of the A18 EPR signal to a C_{1h} symmetry $I\mathrm{O}_i$ defect in the positive charge state.

(submitted to: International Conference in Shallow Level Centers in Semiconductors, Warsaw 2002)
Latex-file available from: Jose Coutinho (coutinho@fis.ua.pt)

Shallow donor activity of S-H, Se-H and Te-H complexes in silicon

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Abstract

The interaction of a single hydrogen atom with a substitutional chalcogen impurity (S, Se or Te) is investigated by *ab-initio* modeling. In Se-H and Te-H complexes, the proton sits at an anti-bonding site relative to a nearest neighbor silicon atom, but two competitive trigonal structures for S-H are found. All the singly hydrogenated complexes are predicted to behave as shallow donors with levels lying above those of the substitutional S, Se and Te double donors. A comparison of our results with experimental data suggests an assignment of the Si-NL60 EPR signal to Se-H.

(submitted to: International Conference in Shallow Level Centers in Semiconductors, Warsaw 2002)
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Numerical computation of critical properties and atomic basins from 3D grid electron densities

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Abstract

InteGriTy is a software package that performs topological analysis following AIM approach on electron densities given on 3D grids. Use of tricubic interpolation is made to get the density, its gradient and hessian matrix at any required position. Critical points and integrated atomic properties have been derived from theoretical densities calculated for the compounds NaCl and TTF-2,5Cl_2BQ, thus covering the different kinds of chemical bonds: ionic, covalent, hydrogen bonds and other intermolecular contacts.

(Submitted to J. Appl. Cryst.)
Manuscripts available from: http://arXiv.org/abs/physics/0205082

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Coulomb Correlations and Magnetic Anisotropy in ordered $L1_0$ CoPt and FePt alloys

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Abstract

We present results of the magneto-crystalline anisotropy energy (MAE) calculations for chemically ordered $L1_0$ CoPt and FePt alloys taking into account the effects of strong electronic correlations and spin-orbit coupling. The local spin density + Hubbard U approximation (LSDA+U) is shown to provide a consistent picture of the magnetic ground state properties when intra-atomic Coulomb correlations are included for both $3d$ and $5d$ elements. Our results demonstrate significant and complex contribution of correlation effects to large MAE of these material.

(Submitted to Phys. Rev. Letters)
Manuscript available from: shick@fzu.cz

^{69,71}Ga NMR Spectra and Relaxation in Wurtzitic GaN

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Abstract

Magnetic properties of wurtzite GaN are studied by Ga nuclear magnetic resonance (NMR) in a GaN bulk crystal containing a high carrier concentration, as well as in highly resistive Mg-doped crystals. The quadrupole coupling constant is derived from the satellite lines and from the shift of the central line in the quadrupolar perturbed ^{69,71}Ga NMR spectra. The electric field gradient is in good agreement with the value calculated by the *ab initio* full-potential linear-muffin-tin-orbital method, using the local density approximation to describe exchange and correlation effects. The ^{69,71}Ga spin lattice relaxations in the Mg-compensated sample in the range 80-400 K are due to the quadrupolar interaction mechanism, similarly to what is observed in GaAs, and the proper scaling factor, given by the square of the ratio of the nuclear quadrupole moments, $(^{69}Q/^{71}Q)^2$, is observed for the two isotopes. In contrast, in the conductive sample the relaxation mechanism is caused by the magnetic interaction with the conduction electrons and one finds a relaxation rate, $W \propto T$. The isotope ratio $^{69}W/^{71}W$ is close to $(^{69}\gamma/^{71}\gamma)^2$, where γ is the gyromagnetic factor. Only above 200 K there is evidence of a relaxation process due to interactions with phonons also in the degenerate sample, with a temperature dependence approximately of the form $W \propto T^3$, consistent with a Debye temperature around 600 K.

(Phys. Rev. B.: submitted)

Manuscripts available from: svane@phys.au.dk

Influence of hydrostatic pressure on cation vacancies in GaN, AlN, and GaAs

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Abstract

The effects of hydrostatic pressure on the formation energy and electronic level positions of cation vacancies in GaN, AlN and GaAs are examined by means of *ab-initio* calculations using a supercell approach in connection with the full-potential linear muffin-tin-orbital method. Atomic relaxations are fully taken into account. Substantial differences are revealed in the pressure behavior of the defect level positions and formation energies for the cation vacancies in the nitride compounds and in GaAs. Additionally, the arsenic antisite in GaAs is examined, also exhibiting pressure response different from that of the vacancies. This effect is strong for the vacancy and the antisite in GaAs, but for similar defects in the III-V nitrides it is rather weak.

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Pressure and composition dependence of the electronic structure of GaAs$_{1-x}$N$_x$.

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Abstract

The electronic band structures of GaAs$_{1-x}$N$_x$ for x =0.016 and 0.031 are calculated *ab initio* using a supercell approach in connection with the full-potential linear muffin-tin-orbital method. The strong nitrogen-induced modification of the conduction band structure is shown. The effects of hydrostatic pressure are examined, and the effective mass of the conduction electrons is studied as a function of pressure and Fermi energy. Strong non-parabolicity is found for the lowest conduction band which leads to an effective mass that increases with the wavenumber. The effect is enhanced with application of pressure, and it further depends on the nitrogen concentration. The theoretical calculations are compared to experimental data, and agreement of general trends is found.

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First principles approach to the electronic structure of strongly correlated systems: combining GW and DMFT

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Abstract

We propose a dynamical mean field approach for calculating the electronic structure of strongly correlated materials from first principles. The scheme combines the virtues of the GW method, namely precise band structure determinations, with the achievements of dynamical mean field theory, which enables one to treat strong interaction effects. It avoids the conceptual problems inherent to conventional "LDA+DMFT", such as the need for Hubbard interaction parameters and double counting terms. We apply a simplified version of the approach to the electronic structure of nickel and find encouraging results.

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Manuscripts available from: Silke.Biermann@lpt.ens.fr
(cond-mat/0207419)

Non-Arrhenius behavior of the island density in metal heteroepitaxy: Co on Cu(001)

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Abstract

We present a combined theoretical and experimental study of island nucleation and growth in the deposition of Co on Cu(001)—a prototype for understanding heteroepitaxial growth involving intermixing. Experimentally, ion scattering is employed. Using density-functional theory, we obtain energy barriers for the various elementary processes and incorporate these into a kinetic Monte Carlo program to simulate the heteroepitaxial growth. Both the simulations and the experiments show a unique "N-shape"-dependence of the island density on temperature that stems from the interplay and competition of the different processes involved.

(Submitted to: Phys. Rev. Lett.)

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Effect of Hydrogen on Al_2O_3/Metal Interfacial Structure and Adhesion

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Abstract

We have carried out an ab initio investigation of the effect of hydrogen on Al_2O_3/Al and Al_2O_3/Cu interfaces. H on the Al_2O_3 surface can play a bridging role in the formation of these interfaces. The surface OH bond is dissociated by as little as a monolayer of Al, while it is stable up to 3 Cu layers. H in the interface significantly lowers the work of separation for both interfaces.

(Submitted to: Phys. Rev. B)

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Half Metallicity Triggers the Electronic Properties of Inverse Magnetoresistant $Fe_{1-x}Co_xSi$ Alloys

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Abstract

Based on *ab-initio* calculations we find that $Fe_{1-x}Co_xSi$ alloys in the Fe-rich region behave as a disordered ferromagnetic half metals, a property of these alloys up to date unknown. Half metallicity can explain the recently found electronic, magnetic and transport properties. We can also determine a sharp transition from the paramagnetic metallic behavior to the ferromagnetic half metallic state as a functions of Co concentration. At concentrations higher than 0.25 the system starts to segregate Co from Fe atoms, this giving rise to the disapearence of half metallicity and reflected in the decreasing magnetic moment.

(Submitted to Phys. Rev. Lett.)
Manuscripts available from: guevara@cnea.gov.ar

Impurity and band effects competition on the appearance of Inverse Giant Magnetoresistance in Cu/Fe multilayers with Cr

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Abstract

We have studied the dependence of impurity *vs.* band effects in the appearance of inverse giant magnetoresistance (IGMR) in Cu/Fe superlattices whit Cr. Current in plane (CIP) and current perpendicular to the plane (CPP) geometries are considered. For the calculation of the conductivities we have used the linearized Boltzmann equation in the relaxation time approximation. Cr impurity effects are taken into account through the spin dependent relaxation times and the band effects through the semiclassical velocities obtained from the LDA calculated electronic structure. The larger the Cr/Fe hybridization strength, the bigger is the tendency towards IGMR. In particular, in CIP geometry roughness at these interfaces increases the IGMR range. The calculated GMR ratios have been compared with the experimental results. From this comparison we conclude that the experimental data can only be explained by taking into account Cr bands.

(Submitted to Phys. Rev. B)
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9 SCIENTIFIC HIGHLIGHT OF THE MONTH

Full-Potential Local-Orbital Minimum-Basis Scheme

FPLO

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Introduction

Every chapter of the well-known textbook *Principles of the Theory of Solids* by J.M. Ziman is headed by a particular quotation. For example, the chapter about *Electronic states* is introduced by R. Kipling's words

> **There are nine and sixty ways of constructing tribal lays,**
> **And-every-single-one-of-them-is-right.**

What Kipling wrote is certainly true. (Who would ever doubt this ?) Also, Ziman took a good choice of the heading, since he intended to emphasize the equivalence of band structure methods **in principle**. Everybody who has been working in our field of electronic structure theory knows, however, that **quantitative** comparisons between recent codes, on a physically relevant scale of accuracy, are still unsatisfactory. This statment does not refer to the never ending discussion if LSDA, GGA, LDA+U, or SIC-LSDA is the preferrable approximation to density functional theory for a given system. What is meant is the purely numerical implementation of a well-defined task. Take six different band structure codes and let them calculate the lattice constant of fcc thorium in LDA. You will get five answers deviating from each other by much more than related experimental data, see Figure 9 in Section . Remember, we do not want to discuss the well-known problem of overbinding in LDA ! ***This problem can only be tackled if we know what the LDA result is.***

At this point it is fair to state that tremendous advances in the numerical techniques have been achieved since John Slater's days. A number of full-potential methods with a high degree of reliability and flexibility have been developed.[1] The price that has to be paid for the accuracy consists of computing time and main storage: linear methods require large basis sets, while non-linear schemes are slow anyway.

Despite the worldwide efforts spent in developing accurate electronic structure code, we are not aware of any reasonable data collection, except that discussed below, comparing the key quantity of DFT, the ground state energy, obtained with essentially different schemes. There is a wide-spread opinion that the numerical accuracy of the codes is more or less unknown. However, if the total energies produced by completely independent codes with tenthousands of command lines would almost coincide, the probability that the codes have noticable errors would be accordingly small.

This highlight is devoted to a recently developed code that provides answeres to both questions raised. The full-potential local-orbital minimum-basis (FPLO) code [1] is

(i) numerically (almost) as efficient as wide-spread lower-accuracy schemes. This efficiency is based on employing a self-adjusting minimum basis. The valence basis is completed by a few upper core states and polarization states.

(ii) The total energy calculated by FPLO coincides with the total energy obtained by the WIEN97 code within chemical accuracy, in the order of 1-2 mHartree per atom. This goal has been achieved by an efficient method to optimize the local basis states with respect to the total energy and by applying a shaping technique for the construction of densities and potentials.

After gathering enough experience with the first version of the code, that has been used and tested by about 10 individuals during the last two years, we decided to release the updated version FPLO®-2. Licences to use this version were issued to 15 groups during the workshop "Hands-on-FPLO" at IFW Dresden, held in the first week of March, 2002. The release includes a fast and convinient user interface and several tools to process output data. Informations on the workshop and on the licence conditions can be obtained from our homepage, **http://www.ifw-dresden.de/FPLO/**.

Before we proceed to present the background of the method and some of the obtained results, a few words should be spent on the history of this development. The ancestor of our present method is the linear combination of atomic orbitals method (LCAO), well-known from textbooks and, besides the complementary plane-wave method, most frequently explained to students in solid state physics. LCAO has two major disadvantages. At first, many Slater-Koster integrals have to be calculated since the atomic functions are far-ranging. Second and more severe, the atomic basis is incomplete if only bound states are included. In the mid-seventies, Helmut Eschrig started to develop an optimized LCAO method being exempt from the mentioned shortcomings. The trick was to smoothly localize the atomic orbitals by an attractive potential [2]. The same idea is used in the present code in refined form, see Section . The ins and outs of

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[1] On purpose, we do not quote the individual methods: to forget one of them would be worse than not to mention any...

Optimized LCAO were published in in the year 1988 together with calculated data for all light metals of the periodic table up to Zn [3].

As time went by, the calculation of band structures and densities of states alone was not sufficient anymore, and total energy calculations came into focus. Optimized LCAO could not compete in this field, since it relied on a representation of radial functions (wave functions, densities, and potentials) in terms of Slater-type orbitals. This choice had been taken on the background of the available main storage (up to at most 1 MByte) of computers accessible to Dresden physicists before 1990. In the early nineteeth, it became clear by attempts of Ulrike Nitzsche that the Slater-type representation had to be abandoned. In addition, we were heading for uttermost accuracy. Thus, Arthur Ernst in our group implemented a mixed basis scheme that achieved this goal at the price of a comparably poor performance [4]. The accuracy obtained by this method is perhaps not surpassed yet, but it cannot be used for elementary cells larger than a few atoms. On the basis of the existing experience, Klaus Koepernik developed the current scheme. It perhaps represents the best compromise between absolute accuracy and performance [1].

The described development through more than two decades was almost from the beginning paralleled by the implementation of important extensions to the basic codes. Chemical disorder could be treated in the optimized LCAO code within non charge-selfconsistent CPA, implemented by the late Reinhard Richter in collaboration with Bedrich Velický [5]. A much extended and completely charge-selfconsistent CPA version [6, 7] was added to FPLO by Klaus Koepernik on the basis of the nearly forgotten pseudo-spin approach of Blackman, Esterling, and Berk. Relativistic versions of both codes have been developed as well, by Manuel Richter for the old code [8, 9] and, quite recently, by Ingo Opahle for FPLO [10]. Both implementations are based on the full four component representation of the Bloch states. Finally, LSDA+U is just about to be completed by Igor Chaplygin.

What remains to be said is organized in the following way. The next section compiles the principles of FPLO in more detail. Sections , , and describe the implementations of CPA, LSDA+U, and the relativistic versions, respectively. The content, the performance, and the portability of the present release, FPLO®-2, are briefly outlined in Section . Finally, Section brings the summary and the outlook.

Principles of FPLO

Local-Orbital Minimum-Basis Scheme

We start from the well-known ansatz for the Bloch states $\psi_{\mathbf{k}n}(\mathbf{r})$,

$$\psi_{\mathbf{k}n}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}\mathbf{s}L} \phi_{\mathbf{s}L}(\mathbf{r}-\mathbf{R}-\mathbf{s}) C_{L\mathbf{s},\mathbf{k}n} e^{i\mathbf{k}(\mathbf{R}+\mathbf{s})} \ . \tag{1}$$

The basis states $\phi_{\mathbf{s}L}$ used to approximate the Kohn-Sham wave function of the crystal are local orbitals centered at sites $\mathbf{s}$ in the elementary cell defined by the lattice vector $\mathbf{R}$. They are solutions of an atom-like Schrödinger equation and are denoted by a complete set of atomic quantum numbers $L = \{\rho, l, m\}$.

The secular equation to be solved is

$$HC = SC\epsilon\ , \tag{2}$$

since the basis is nonorthogonal. Hamiltonian and overlap matrices are defined according to

$$H_{\mathbf{s}'L',\mathbf{s}L} = \sum_{\mathbf{R}} \langle \mathbf{0}\mathbf{s}'L'|\hat{H}|\mathbf{R}\mathbf{s}L\rangle e^{i\mathbf{k}(\mathbf{R}+\mathbf{s}-\mathbf{s}')}, \tag{3}$$

$$S_{\mathbf{s}'L',\mathbf{s}L} = \sum_{\mathbf{R}} \langle \mathbf{0}\mathbf{s}'L'|\mathbf{R}\mathbf{s}L\rangle e^{i\mathbf{k}(\mathbf{R}+\mathbf{s}-\mathbf{s}')}. \tag{4}$$

As usual, the local basis states are divided into two classes, the core states $\phi_{\mathbf{s}L_c}$ and the valence states $\phi_{\mathbf{s}L_v}$, to avoid unnecessarily large matrix problems. We define the core states by

$$\langle \mathbf{R}'\mathbf{s}'L_c'|\mathbf{R}\mathbf{s}L_c\rangle = \delta_{cc'}\delta_{\mathbf{R}\mathbf{R}'}\delta_{\mathbf{s}\mathbf{s}'}\ . \tag{5}$$

Provided this condition is fulfilled (in practice, to the requested level of accuracy), the core states can be removed from the basis by an exact transformation [4]. At first, we decompose the overlap matrix,

$$S = \begin{pmatrix} 1 & S_{cv} \\ S_{vc} & S_{vv} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ S_{vc} & S_{vv}^{L} \end{pmatrix} \begin{pmatrix} 1 & S_{cv} \\ 0 & S_{vv}^{R} \end{pmatrix} = S^L S^R, \tag{6}$$

where left and right triangular matrices S_{vv}^L and S_{vv}^R obey the relation

$$S_{vv}^L S_{vv}^R = S_{vv} - S_{vc}S_{cv}\ . \tag{7}$$

Further, by definition of the core states,

$$H = \begin{pmatrix} \epsilon_c 1 & \epsilon_c S_{cv} \\ S_{vc}\epsilon_c & H_{vv} \end{pmatrix}, \quad \epsilon_c = \mathrm{diag}(\cdots, \epsilon_{\mathbf{s}L_c}, \cdots). \tag{8}$$

Re-writing the secular equation,

$$(S^L)^{-1} H (S^R)^{-1} (S^R C) = (S^R C)\epsilon \tag{9}$$

leads us finally to the reduced problem

$$\tilde{H}_{vv}\tilde{C}_{vv} = \tilde{C}_{vv}\epsilon_v\ , \tag{10}$$

with the definition

$$\tilde{H}_{vv} = (S_{vv}^L)^{-1}(H_{vv} - S_{vc}H_{cc}S_{cv})(S_{vv}^R)^{-1} \tag{11}$$

and

$$C = \begin{pmatrix} 1 & -S_{cv}(S_{vv}^R)^{-1}\tilde{C}_{vv} \\ & \\ 0 & (S_{vv}^R)^{-1}\tilde{C}_{vv} \end{pmatrix}\ . \tag{12}$$

The orthogonality condition for the core states is controlled during the successive iterations and related warnings or error messages are displayed.

Basis Optimization

A crucial feature of the method is that the basis is readjusted at every iteration cycle and is optimized in the course of iteration. The core states obey the equation

$$\left(\hat{t} + v_{\mathbf{s}}^{\mathrm{at}}\right) \phi_{\mathbf{s}L_c} = \phi_{\mathbf{s}L_c} \epsilon_{\mathbf{s}L_c} \tag{13}$$

with $v_{\mathbf{s}}^{\mathrm{at}}$ being the crystal potential spherically averaged around the site center $\mathbf{s}$. The latter definition assures that a Bloch sum of the core orbitals and the related core eigenvalues $\epsilon_{\mathbf{s}L_c}$ are very good approximations to the solution of the true crystal Hamiltonian.

On the contrary, the valence orbitals are defined in the following way:

$$\left(\hat{t} + v_{\mathbf{s}}^{\mathrm{at}} + \left(\frac{r}{r_{\mathbf{s}L_v}}\right)^4\right) \phi_{\mathbf{s}L_v} = \phi_{\mathbf{s}L_v} \epsilon_{\mathbf{s}L_v} \tag{14}$$

with $r_{\mathbf{s}L_v} = (r_{\mathrm{NN}}(\mathbf{s}) x_{0L_v}/2)^{\frac{3}{2}}$, where r_{NN} is the nearest neighbor distance and x_{0L_v} are dimensionless compression parameters. The seemingly strange scaling of the $r_{\mathbf{s}L_v}$ is the correct one for an empty lattice.

The effect of the additional confining potential is to compress the long-ranging orbital tails of the valence orbitals. The power law potential has minor influence on the orbital in the core region, while in the region far from the nucleus the orbitals undergo a drastic change, compared to solutions without the confining potential. To be precise, the valence orbitals are usually unbound states in the potential $v_{\mathbf{s}}^{\mathrm{at}}$ alone. A second, even more important effect of the valence orbital confinement is that the orbital resonance energies are pushed up to come close to the band centers, providing the optimum curvature of the orbitals (Figure 1).

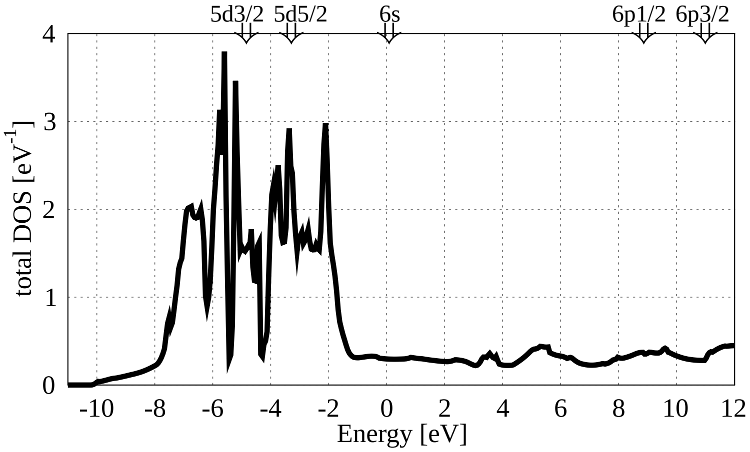

Figure 1: Total density of states of Au and the orbital energy positions $\epsilon_{\mathbf{s}L_v}$ of the optimized local basis states. All energies are relative to the Fermi level. (This figure has been produced with the relativistic FPLO code.)

The parameters x_0 enter the total energy via the basis expansion of the valence eigenstates. Therefore, the total energy is depending on x_0 as long as the basis set is incomplete. The most important feature of the FPLO basis treatment is that the total energy is minimized with respect to the set of compression parameters. In consequence, FPLO is not a fixed basis scheme.

In the self consistent calculation, the basis is adapted to the best x_0 set by using relations similar to the force theorem. One can prove the equality

$$\partial_{x_0} E^{\mathrm{tot}} = \sum_{\mathbf{k}n}^{\epsilon_F} \partial_{x_0} \epsilon_{\mathbf{k},n} - \int n(\mathbf{r}) \partial_{x_0} V^{cr}(\mathbf{r}) d\mathbf{r} \tag{15}$$

using $\partial_{x_0} N = \int \partial_{x_0} n(\mathbf{r}) d\mathbf{r} \equiv 0$. The right-hand side of Eq. (15) turns out to be exactly zero for all x_0 if the basis orbitals form a complete set. Since the latter is obviously not the case, we require $\partial_{x_0} E^{\mathrm{tot}}$ to vanish and obtain matrix equations for the calculations of the compression parameters, which then are solved simultaneously with the Kohn-Sham equations in every iteration step. This method turns out to be very efficient. A rule of thumb is that, depending on the starting values for x_0, a calculation with basis optimization takes only $1.5 \ldots 3$ times more iterations than without.

Partitioning of unity and shape functions

The representation of density and potential as locally finite lattice sums is achieved by using the partitioning of unity. Two types of shape functions are employed in FPLO.

(i) The overlap density is a lattice sum of terms, consisting of a product of two orbitals located at different lattice sites with a generalized occupation number. These terms have two cusps, one at each site. Each term is split into contributions from the two sites, which are “localized” at the corresponding site and fall off to zero at the other:

$$\phi_i n_{ij} \phi_j = f_{ij}(\mathbf{r}) \phi_i n_{ij} \phi_j + \phi_i n_{ij} \phi_j f_{ji}(\mathbf{r}) \ , \tag{16}$$

using 1D shape functions f_{ij} with the following properties

- $f_{ij}(\mathbf{r}) + f_{ji}(\mathbf{r}) \equiv 1 \quad \forall \mathbf{r}$
- $f_{ij}(\mathbf{s}_i) = f_{ji}(\mathbf{s}_j) = 1$
- f_{ij} is continuously differentiable to a certain degree
- f_{ij} behaves like $1 - O(|\mathbf{r} - \mathbf{s}_i|^N)$ and $O(|\mathbf{r} - \mathbf{s}_j|^N)$ at the site i and j respectively, with a certain order N

These properties assure that the function at one site will screen the cusp at the other site in a controlled manner.

One possible choice of shape functions is:

$$f_{ij}(\mathbf{r}) = p(x), \quad f_{ji}(\mathbf{r}) = p(1-x) \tag{17}$$

with $x = (\mathbf{r} - \mathbf{s}_i)(\mathbf{s}_j - \mathbf{s}_i)/|\mathbf{s}_j - \mathbf{s}_i|^2$ and $p(x) + p(1-x) \equiv 1$, $p(x) \equiv 1 \ \ \forall \ \ x \leq 0$ and $p(x) \equiv 0 \ \ \forall \ \ x \geq 1$. For the profile function $p(x)$ one may chose any function which fulfills

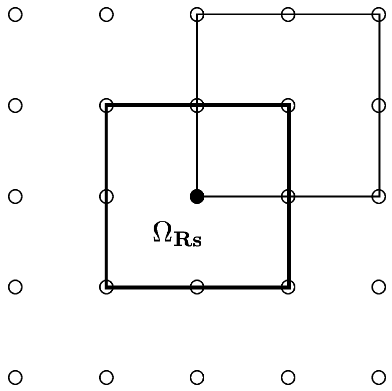

Figure 2: Overlapping Voronoi cells in a 2D square lattice.

the differentiability and power law conditions given above. Any such function creates a class of similar functions, generated by $p_n(x) = p(1 - p_{n-1}(x))$.

(ii) For the decomposition of the non-linear exchange and correlation potential into a sum of locally finite contributions we use a 3D shape function. The requirements for this functions are

- Each single shape function $f_i(\mathbf{r})$ is centered at a certain site $\mathbf{s}_i$
- $\sum_i f_i(\mathbf{r}) \equiv 1 \quad \forall \mathbf{r}$
- $f_i(\mathbf{r} - \mathbf{s}_i) \equiv 1 - O((\mathbf{r} - \mathbf{s}_i)^N)$
- The shape function at $\mathbf{s}_i$ (when multiplied with a lattice symmetric function) screens the singularities at all other lattice sites $\mathbf{s}_j$:
  $f_i(\mathbf{r} - \mathbf{s}_j) \equiv 0 + O((\mathbf{r} - \mathbf{s}_j)^N) \quad \forall j \neq i$
- f_i is continuously differentiable to a certain degree.
- The shape function has the "smallest possible compact support".

Our choice of shape functions is defined as follows. The most compact supports, which may be defined for every site in an arbitrary lattice are the Voronoi cells. Since the resulting shape functions should be overlapping, we chose Voronoi cells Ω with an eightfold volume compared to the standard definition. The distance between the central site and the defining boundary planes is two times larger than usual. Figure 2 shows overlapping Voronoi cells according to our definition in a 2D square lattice.

Each cell-defining plane is related to a certain neighboring site $\mathbf{s}_j$. For a given site $\mathbf{s}_i$, we define dimensionless scalar variables x_j and 1D profile functions h_j for every neighboring site $\mathbf{s}_j$, contributing to the cell boundary definition:

$$h_j(\mathbf{r}) = p(x_j), \quad x_j = \frac{(\mathbf{r} - \mathbf{s}_i)(\mathbf{s}_j - \mathbf{s}_i)}{|\mathbf{s}_j - \mathbf{s}_i|^2} \tag{18}$$

with an appropriately chosen profile $p(x)$:

- $p(0+\delta) \equiv 1 - O(\delta^N)$
- $p(1-\delta) \equiv 0 + O(\delta^N)$
- $p(x)$ continuously differentiable to a certain degree and monotonously decreasing
- $p(x) = 0, \quad x \geq 1$
- $p(x) = 1, \quad x \leq 0$

The product of all profile functions gives a cell-function

$$g_i(\mathbf{r}) = \prod_{\{j\}} h_j(\mathbf{r}) \;, \tag{19}$$

which excludes by its definition every lattice site except $\mathbf{s}_i$. Additionally, it falls off faster than a given power law, when approaching the cell boundary (and thus a neighbor site). The unity condition for the lattice sum of all shape functions is achieved by explicit normalization. Thus, the shape function reads

$$f_i(\mathbf{r}) = \frac{g_i(\mathbf{r})}{\sum g_i(\mathbf{r})} \;, \tag{20}$$

where the sum runs over all neighboring sites whose Voronoi cells overlap the cell at site $\mathbf{s}_i$. This is always a finite sum and it turns out that the numerical implementation of the shape functions described above is extremely efficient.

Density and Potential representation

Details of density and potential calculation have been published elsewhere [1]. Thus, we concentrate on the key points here.

The (spin) density in a non-orthogonal local basis scheme consists of net and overlap contributions. The former terms contain products of basis functions from the same site and are site-centered by construction. The latter terms contain products of basis functions from different sites. They are decomposed into site-centered contributions by application of the described partitioning technique. As a result, the total density is obtained as a lattice sum of site densities in spherical harmonics representation,

$$n(\mathbf{r}) = \sum_{\mathbf{R}\mathbf{s},lm} n_{\mathbf{s},lm}(|\mathbf{r}-\mathbf{R}-\mathbf{s}|)Y_{lm}(\mathbf{r}-\mathbf{R}-\mathbf{s}) \;. \tag{21}$$

The maximum l-numbers used are 6 for the net contributions (by construction from states of $l_{\max} = 3$) and 12 for the overlap contributions.

The Hartree potential is evaluated with the help of Ewald's method applied to all multi-pole components. While the local part can be used 'as is', the Fourier-transformed contribution is inserted into the 3D partitioning-mill described in the previous section. This again provides us with a locally finite lattice sum. Finally, the xc potential is partitioned in exactly the same way, and the local contributions to the crystal potential are expanded into spherical harmonics,

$$V^{cr}(\mathbf{r}) = \sum_{\mathbf{R}\mathbf{s},lm} v_{\mathbf{s},lm}(|\mathbf{r}-\mathbf{R}-\mathbf{s}|)Y_{lm}(\mathbf{r}-\mathbf{R}-\mathbf{s}) \;. \tag{22}$$

Now, when it comes to evaluate the multi-center Slater-Koster integrals, we can joyfully harvest the fruits of our endeavors. As the extension of all involved functions is finite and restricted to few neighbor atoms, relatively few integrals have to be calculated, and no cut-off is needed. The one- and two-center integrals are further simplified by the application of angular momentum rules to one- and two-dimensional numerical integrations, respectively. All integration meshes are tuned to achieve accuracies of better than 1 μHartree in the Hamiltonian integrals and better than 10^{-6} in the overlap integrals.

Coherent Potential Approximation (CPA) for partial substitutional disorder

The density- and potential representation as well as the local orbital basis set used in FPLO are well suited to apply a variant of the CPA to describe disordered bulk materials. For this purpose we employ a generalization of the Blackman-Esterling-Berk (BEB) matrix-CPA. This version of CPA provides a scattering theory in matrix notation, which parallels the usual KKR-formulation. In contrast to all other simple types of matrix CPA, the BEB-CPA does not restrict the values of the Hamiltonian matrix elements. It completely incorporates the off-diagonal disorder effects. Moreover, the BEB-CPA has been proven to fulfill the dilute or single impurity limit.

The main ingredients and approximations are sketched in the following. The random occupation of the lattice sites is described by assigning pseudo spins to every site, labeled by the atom sorts, which may occupy the site under consideration. They take values 1 or 0, depending on the occupation of the site. This treatment is flexible and allows the description of partial disorder. We assume statistical independence of pseudo spins from different sites, thus neglecting short range order effects.

The main assumption is the linear dependency of all real space functions (density, potential, and orbitals) on the pseudo spins. In this way it is possible to write down density, potential, Hamiltonian, and Green's function as pseudo spin dependent random objects, which model a statistical ensemble. For a certain member of the ensemble, say a particular realization of all pseudo spins, these objects become nonrandom and represent the behavior of exactly this member.

The random Hamiltonian and Green's matrix are defined in an enlarged Hilbert space (due to the pseudo spin degrees of freedom), which to a certain extent describes the true statistical ensemble. The equation of motion for the Green's function is formulated in this Hilbert space. One can write down the scattering matrix for this equation and ends up with a CPA condition, which defines an averaged Green's matrix in the enlarged space. It is possible to show, that the matrix elements of this averaged Green's function represent relevant partially averaged physical quantities like generalized occupation numbers, which enter the density expression.

In practical calculations, the CPA condition is solved within the single site approximation (the scattering matrix is decoupled into single site events and the CPA-condition is applied to the single site scattering matrices only). The second simplification is done for the occupation numbers entering the density expression. It is assumed, that the true (random) occupation numbers may be replaced by conditional averages with only the sites indexing the occupation numbers being kept random. The resulting density expression is again linearly depending on the pseudo spins and, thus, all ingredients for a charge self-consistent calculation are defined.

The CPA method, as shortly outlined above, has been applied to the FeAl system. This system undergoes several structural and magnetic phase transitions in dependence of concentration and temperature. The iron rich site of the phase diagram consists of structures, derived from the bcc structure. All atoms are at bcc sites, but the occupation is partially disordered (experiments provide evidence for partial long range order). Depending on the actual occupation one may describe the resulting structures by superstructures of the bcc lattice, where some sub-lattices are occupied with iron or aluminum only, while the other sub-lattices may be occupied randomly by iron and aluminum. Three possible structures are the A_2 structure (completely disordered bcc lattice), the B_2 structure (CsCl structure with one sub-lattice randomly occupied), and the DO_3 structure (four sub-lattices, one or two occupied randomly, depending on the aluminum concentration.)

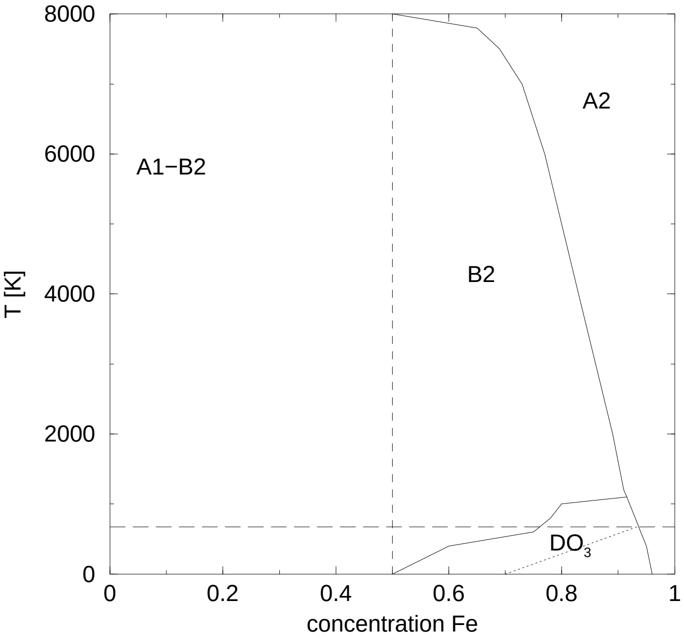

Figure 3: Theoretical phase diagram of Fe-Al.

We have investigated the influence of the types of partial disorder on the magnetic and mechanical properties. For every structure type and concentration we optimized the lattice constant. The resulting energy surface was combined with a simple mixing entropy term to provide an estimate for the enthalpy. From this we concluded a rough picture of the phase diagram at the iron rich side, Figure 3. In the Fe concentration range $50\% - 96\%$ the DO_3 phase has the lowest enthalpy at low T. Above 90% Fe, the A_2 phase replaces the DO_3 phase when temperature increases, while below 90% Fe concentration, the DO_3 phase is replaced by the B_2 phase. Above 70% the enthalpy curve is concave, which indicates de-mixing and instability of the DO_3 and B_2 phases.

Experiments indicate only a small concentration region around 70% Fe, where a DO_3 like phase is stable. This contradicts our finding of a stable DO_3 phase extending over a larger concentration range. We believe that the experimentally observed B_2 phase is a thermodynamically metastable phase, resulting from freezing of atom exchange when cooling down the sample. On the other hand, the enthalpy difference between B_2 phase and DO_3 phase becomes rather small for concentrations close to 50% Fe.

There are other quantities supporting the stability of the DO_3 phase found in our calculation. The first result concerns the equilibrium volume at zero temperature. Starting from pure iron, the lattice volume is linearly increasing with the aluminum concentration. Around 70% Fe the volume stays more or less constant while for still lower Fe concentrations the volume is further increasing. This behavior is exactly reproduced in the spin polarized DO_3 phase calculations. The reason for this finding is a magneto-strictive effect. In the same region where the lattice constant is staying constant the magnetic moment strongly decreases with increasing Al content. We have found two minima in the total energy versus the magnetic moment. Depending on the lattice constant, one of the two minima is stable. This could provide a simple mechanism of magneto-striction. As a final note, the B_2 phase shows similar behavior, but the DO_3-phase magnetization and volume versus concentration curves are resembling the experimental findings more closely.

LSDA+U

We have implemented the LSDA+U approximation for computing the electronic structure of compounds with strong correlations, such as transition metal oxides. It is well known that LSDA often fails to describe the transport and magnetic properties of such compounds. The reason for this failure is primarily an insufficient description of the on-site Coulomb correlation of the d-electrons. LSDA+U proves to give better results in many cases.

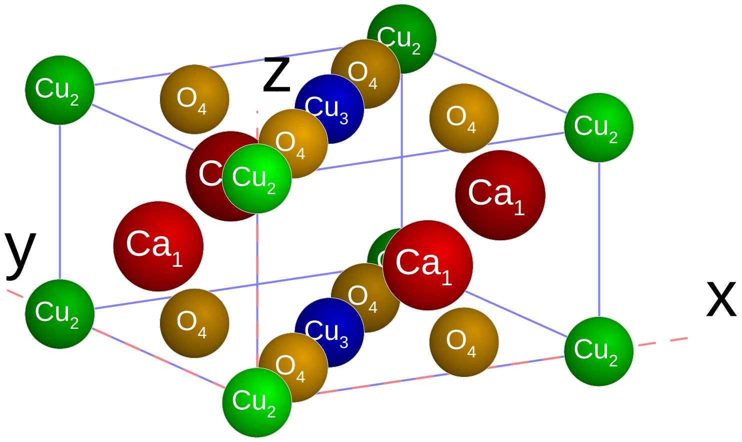

Figure 4: Antiferromagnetic unit cell of $CaCuO_2$. Note that the cell is rotated by $\pi/4$ about the Z-axis with respect to the standard CuO_2 plaquett, so that the d_{xy} copper orbital is involved in σ-bonding with in-plane p-orbitals of the neighboring oxygen atoms.

The implemented version of LSDA+U is rotationally invariant and has few free parameters (Slater integrals). In the considered d-systems, we restrict the number of parameters to the Coulomb U and exchange J interaction constants. Under fixed choice of the parameters and well-defined d-orbitals the LSDA+U ground-state energy is a functional of spin-density, which puts a rigorous ground for using it in the framework of DFT. The chosen form of the double-counting term ensures that the functional reduces to that of LSDA in the limiting cases of full or zero occupation of the relevant shell.

As an example, results for the compound $CaCuO_2$ are presented. This compound does not exist in nature in the pure form but can be stabilized by substituting about 14% of Ca by Sr. The idealized crystal $CaCuO_2$ has simple tetragonal structure and is made up of CuO_2 planes separated by Ca layers. The elementary cell of $CaCuO_2$ with chessboard-ordered antiferomagnetic arrangement is shown in Fig. 4. The lattice constants $a = 5.46$ Å and $c = 3.20$ Å were used in the calculations.

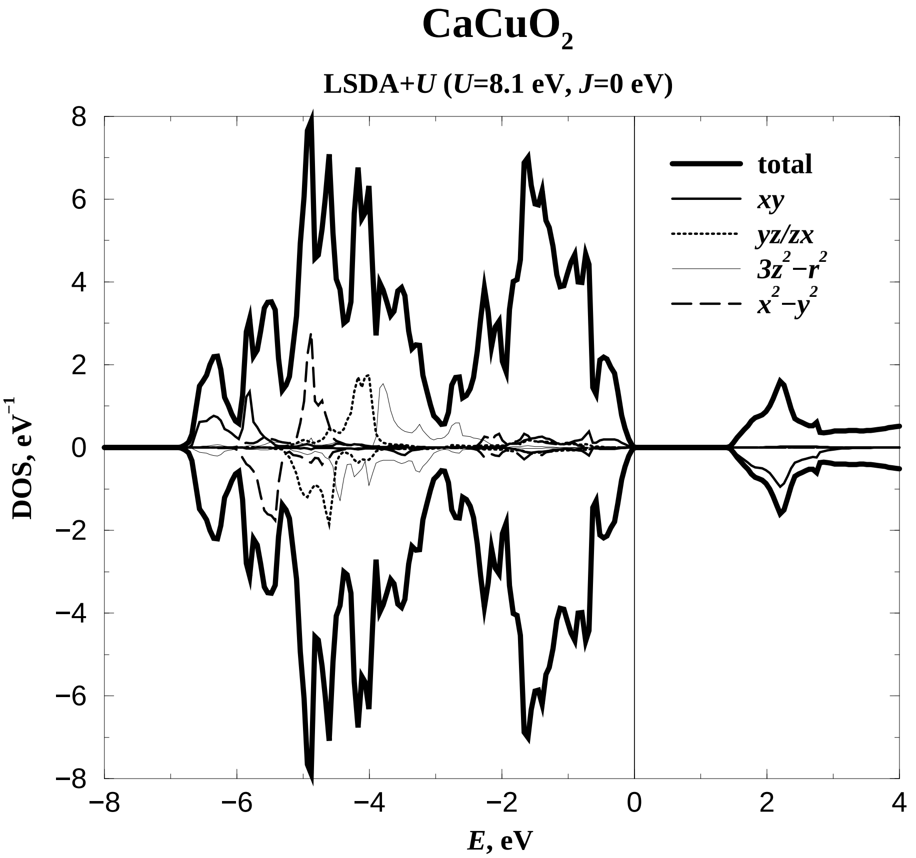

Figure 5: Density of states of antiferromagnetic $CaCuO_2$ projected on d-orbitals of a copper atom. The majority and minority spin channels are drawn above and below the X-axis, respectively. Empirical values $U = 8.1$ eV and $J = 0$ eV are used.

LSDA predicts the compound to be a paramagnetic metal, though its existing counterpart $Ca_{0.86}Sr_{0.14}CuO_2$ is an antiferromagnet with large insulating gap, the influence of the Sr substitution impurity on the electronic structure being negligible.

The implemented LSDA+U version yields the correct insulating ground state. The values of the magnetic spin moment, 0.71 μ_B per Cu atom, and the width of the gap, 1.44 eV, are close to the experimental values (total moment 0.51 μ_{B} per Cu atom and gap width 1.5 eV). The computed density of states projected on d orbitals of a copper atom is shown in Fig. 5. One notes that one d_{xy}-orbital ($d_{x^2-y^2}$ in standard notation) is unoccupied and split off the rest Cu-3d/O-2p complex.

Relativistic Versions

Four component relativistic FPLO

Our aim is to solve the Kohn-Sham-Dirac equation in local spin density approximation (LSDA),

$$\hat{H}|\mathbf{k}n\rangle = \left[-ic\alpha\nabla + \beta c^2 + V^{cr} + \beta\Sigma_z B^{cr}\right] \, |\mathbf{k}n\rangle = \epsilon|\mathbf{k}n\rangle \ , \tag{23}$$

with the XC-field $\mathbf{B} \equiv B^{cr}\hat{z}$ treated in a collinear approximation and aligned along the (arbitrary) $\hat{z}$-axis,

$$B^{cr}(\mathbf{r}) = \frac{1}{2}\left(V_{xc}^{+}[n,m] - V_{xc}^{-}[n,m]\right) \ . \tag{24}$$

As usual, the effective crystal potential, V^{cr}, in equation (23) contains the Hartree potential, the external potential V and the exchange and correlation potential V_{xc},

$$V^{cr}(\mathbf{r}) = \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d^3r' - \sum_{\mathbf{Rs}} \frac{Z_{\mathbf{s}}}{|\mathbf{r}-\mathbf{R}-\mathbf{s}|} + \frac{1}{2}\left(V_{xc}^{+}[n,m] + V_{xc}^{-}[n,m]\right) \ . \tag{25}$$

Further, c denotes the velocity of light, and α, β and Σ_z are the usual 4×4 Dirac and Pauli matrices. In contrast to most other relativistic band structure methods we solve equation (23) in a four component formalism, thus avoiding further approximations like the second variation treatment.

The scheme presented here is a relativistic extension of the non relativistic FPLO scheme described in Section 2 and is built on the same numerical grounds, thus enabling us to study the influence of relativistic effects within one and the same highly accurate scheme. To stress this opportunity, we mention that the total energies obtained by the non relativistic FPLO code and by the RFPLO code in a quasi non relativistic mode ($c = 10^6$) agree within some μHartree even for heavy elements like Au, with the main deviations stemming from the 1s electrons. The scalar relativistic implementation (SRFPLO) is briefly described in the second part of this section.

The same kind of ansatz for the Bloch states as in the non relativistic version is used,

$$|\mathbf{k}n\rangle = \sum_{\mathbf{Rs}\nu} \frac{1}{\sqrt{N}} C_{\nu\mathbf{s},\mathbf{k}n} \, |\mathbf{Rs}\nu\rangle \, e^{i\mathbf{k}(\mathbf{R}+\mathbf{s})} \ , \tag{26}$$

but now in terms of localized four-spinors $|\mathbf{Rs}\nu\rangle$. The label $\nu = (\rho, \kappa, \mu)$ denotes a complete set of atomic quantum numbers in relativistic notation. The chosen ansatz includes only electron-like spinors with the ratio between large and small components determined in the preceding solution of atomic-like problems. This ensures (i) minimum size of the matrix, namely twice the size of the non relativistic problem and (ii) a restriction of the solutions to the electron sector of the Hilbert space.

For our minimum basis scheme, the optimum choice of the local basis states $|\mathbf{R}\mathbf{s}\nu\rangle$ is crucial for highly accurate and efficient calculations. In analogy to the non relativistic FPLO scheme, we define the local basis states as solutions of a single particle Dirac equation

$$\left[-ic\alpha\nabla + \beta c^2 + v^{at}_{\mathbf{s}\nu} + \beta\Sigma_z B^{at}_{\mathbf{s}\nu}\right]\ \phi_{\mathbf{s}\nu} = \pm\phi_{\mathbf{s}\nu}(\epsilon_{\mathbf{s}\nu} + c^2) \tag{27}$$

in a spherical, orbital dependent potential

$$v^{at}_{\mathbf{s}\nu}(|\mathbf{r}-\mathbf{s}|) = v^{at}_{\mathbf{s}}(|\mathbf{r}-\mathbf{s}|) + V^{\mathrm{conf}}_{\rho l} = \frac{1}{4\pi}\int d\Omega\, V^{cr}(\mathbf{r}-\mathbf{s}) + \delta_{\nu v}\frac{1+\beta}{2}\left(\frac{|\mathbf{r}-\mathbf{s}|}{r_{0,\rho l}}\right)^4 \tag{28}$$

which is the sum of the spherically averaged crystal potential, $v^{at}_{\mathbf{s}}$, and an additional confining potential term that is only applied to valence states (denoted by the symbolic writing $\delta_{\nu v}$). Further, the spherically averaged crystal XC-field is included,

$$B^{at}(|\mathbf{r}-\mathbf{s}|) = \frac{1}{4\pi}\int d\Omega\, B^{cr}(\mathbf{r}-\mathbf{s}). \tag{29}$$

For the solution of equation (27) we neglect the magnetic coupling terms of order $O(1/c^2)$ [11] and take an ansatz

$$\phi_{\rho\kappa\mu}(\mathbf{r}) = \begin{pmatrix} g_{\rho\kappa\kappa\mu}(r)\chi_{\kappa\mu}(\hat{r}) \\ if_{\rho\kappa\kappa\mu}(r)\chi_{-\kappa\mu}(\hat{r}) \end{pmatrix} + \begin{pmatrix} g_{\rho\kappa\tilde{\kappa}\mu}(r)\chi_{\tilde{\kappa}\mu}(\hat{r}) \\ if_{\rho\kappa\tilde{\kappa}\mu}(r)\chi_{-\tilde{\kappa}\mu}(\hat{r}) \end{pmatrix} \tag{30}$$

with $\tilde{\kappa} = -\kappa - 1$ and spherical spinors

$$\chi_{\kappa\mu}(\hat{r}) = \begin{pmatrix} c_{\kappa\mu\uparrow}\mathcal{Y}_{l_\kappa\mu-\frac{1}{2}}(\hat{r}) \\ c_{\kappa\mu\downarrow}\mathcal{Y}_{l_\kappa\mu+\frac{1}{2}}(\hat{r}) \end{pmatrix} \tag{31}$$

where the $\mathcal{Y}_{lm}$ are complex spherical harmonics and the $c_{\kappa\mu\sigma}$ are Clebsch-Gordan coefficients. This ansatz gives rise to a set of four coupled differential equations, except for the case $|\mu| = l_\kappa + \frac{1}{2}$. In the case of a non magnetic calculation, the ansatz (30) reduces to

$$\phi_{\rho\kappa\mu}(\mathbf{r}) = \begin{pmatrix} g_{\rho\kappa}(r)\,\chi_{\kappa\mu}(\hat{r}) \\ if_{\rho\kappa}(r)\,\chi_{-\kappa\mu}(\hat{r}) \end{pmatrix} \tag{32}$$

giving rise to two coupled equations. For both types of equations, a number of numerical standard methods exist, such as Runge-Kutta or multi step methods. We use a predictor corrector method of Adams-Bashford-Moulton type.

The numerical effort of a local-basis method is determined by the size of the matrix on the one hand, and by the number of multi center integrals on the other hand. We have already discussed the matrix size, being twice as large as in the non relativistic approximation. For small elementary cells and moderate numbers of **k** points, however, the numerical effort is primarily determined by the multi center integrals. Given a certain geometry, it depends mainly on the number of different radial functions we have to consider. Consider at first non magnetic calculations. Here, we have roughly twice the number of radial functions for the large components (due to the $j = l \pm \frac{1}{2}$-splitting of states with $l > 0$) compared to the non relativistic approach, enhancing the effort to calculate Slater-Koster integrals by a factor of $3\dots4$. The same holds true for the small components, giving another factor of two for the total effort. This is still tractable and *can also be done with the actual RFPLO code.*

However, in standard calculations we take advantage of the fact that the small components are virtually *confined within half of the nearest neighbor distance*, so that we can neglect all the multi center integrals between small components. With this approximation we save a factor of two both in the calculation time and memory, while allowing for a tiny error in the absolute value of the total energy. It is of the order of 50 μHartree per atom for gold, much smaller than our accuracy demands (Figure 6).

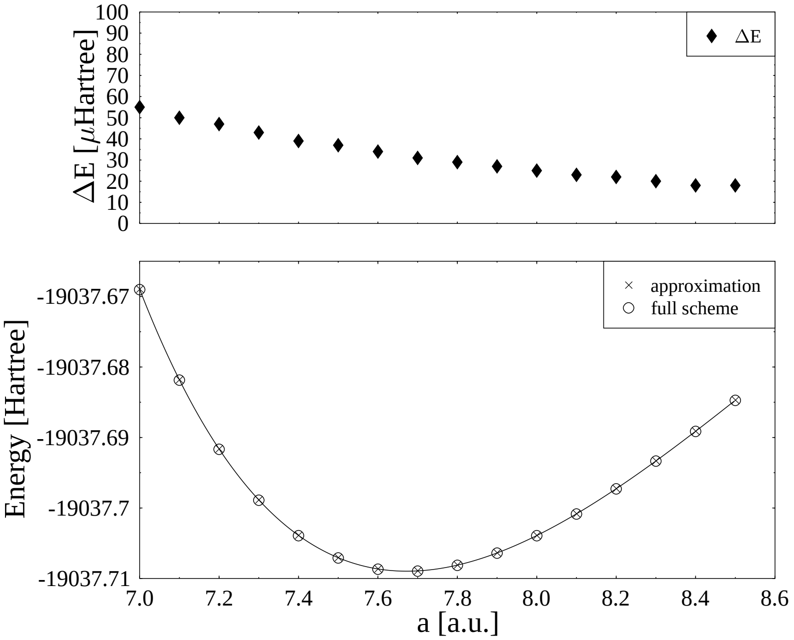

Figure 6: Total energy of Au versus lattice constant, using the Perdew-Wang 92 version of LDA and a minimum valence basis including 5p, 6s, 6p, and 5d states. Results obtained by including and excluding the overlap between small components on different sites are compared. The related energy difference is shown in the upper panel at enlarged scale.

In the case of magnetic calculations, the method is tedious if no additional approximations are made. For a d-shell, e.g., there are ten states with different energies, each of them having two different radial wave functions (except for the $\mu = \pm\frac{5}{2}$-states) for the large components. Taking into account the small components as well, we easily arrive at a factor of 10^3 for the numerical effort, in comparison with the non relativistic situation. We thus introduce the following approximative scheme which also allows calculations for more complicated structures with an acceptable accuracy. Again, the code allows to switch off the described approximation to allow full control of the accuracy at the price of enhanced computational effort.

For each (ρ, l)-shell the radial functions of the large components are approximated by a linear combination of two radial functions

$$g_{\rho\kappa\mu\sigma} \approx c_{\rho\kappa\mu\sigma} g_{\rho l} + \tilde{c}_{\rho\kappa\mu\sigma} \tilde{g}_{\rho l}. \tag{33}$$

This approach is exact in the two limiting cases of vanishing spin polarization or vanishing spin-orbit interaction. The coefficients $c_{\rho\kappa\mu\sigma}$ and $\tilde{c}_{\rho\kappa\mu\sigma}$ are determined in such a way that the expression

$$||g_{\rho\kappa\mu\sigma} - (c_{\rho\kappa\mu\sigma} g_{\rho l} + \tilde{c}_{\rho\kappa\mu\sigma} \tilde{g}_{\rho l})|| \tag{34}$$

is minimized. For the functions $g_{\rho l}$ and $\tilde{g}_{\rho l}$ we take the (normalized) radial wave functions of the large components belonging to the state with the highest and lowest energy of the specific (ρ, l)-shell. The scheme is written quite general, so that an approximation with a larger set of functions would not pose any problem. In all cases tested so far, the influence of the present approximation on the total energies was well below 100 μHartree per atom. The effect on relative energy differences like magneto-crystalline anisotropy energies (MAE) is tiny and can be neglected in comparison with other sources of errors like the finite **k**-mesh. This insensitivity is reasoned by the little effect of a rotation of magnetization direction on the size of the spin moment (apart from heavy elements, where the MAE is large).

Scalar Relativistic FPLO

For many applications, an approximate consideration of relativistic effects is sufficient. Spin-orbit coupling is neglected in so-called scalar relativistic approaches, so that wave functions with non-relativistic symmetry are obtained. There is, however, no unique definition of a scalar relativistic approximation possible. Frequently used schemes are those due to Koelling and Harmon [12] or Douglas, Kroll, and Hess, employed in Reference[13].

Our approach does not rely on solving an explicit scalar-relativistic equation but rather on averaging the large components and related energies of the local orbitals. It was previously implemented in the relativistic OLCAO method [8]. The advantage over other scalar relativistic schemes is an enhanced accuracy of the charge density close to the atomic nuclei and a smaller difference of the total energy from fully relativistic calculations.

Neglecting spin dependence for the sake of simplicity, we define scalar relativistic local basis states $|\mathbf{Rs}L)$ by

$$\tilde{H}^{at}\,|\mathbf{Rs}L) = \tilde{\epsilon}_{\mathbf{s}\rho l}\,|\mathbf{Rs}L) \tag{35}$$

$$(\mathbf{r}|\mathbf{Rs}L) = f_{\mathbf{s}\rho l}(r)\,Y_{lm}(\hat{r}) \tag{36}$$

as solutions of a fictitious spherical Hamiltonian $\tilde{H}^{at}$ with non-relativistic symmetry. The scalar relativistic radial wave functions

$$f_{\mathbf{s}\rho l}(r) = \frac{1}{\mathcal{N}} \sum_{j=l\pm\frac{1}{2}} \sum_{\mu=-j}^{j} g_{\mathbf{s}\rho\kappa(j)}(r) \tag{37}$$

are defined by averaging over the large components of all states of a (ρ, l)-shell, with a normalization factor $\mathcal{N}$. The scalar relativistic one particle energies

$$\tilde{\epsilon}_{\mathbf{s}\rho l} = \frac{1}{4l+2} \sum_{j=l\pm\frac{1}{2}} \sum_{\mu=-j}^{j} \epsilon_{\mathbf{s}\rho\kappa(j)} \tag{38}$$

are also averaged over the spin orbit split energies of a (ρ, l)-shell. The scalar relativistic Hamiltonian $\tilde{H}^{at}$ is defined only implicitly by Eqs. (35), (37) and (38).

The remaining treatment of the valence states completely parallels the non-relativistic version, while core states are treated in the same way as in a relativistic calculation.

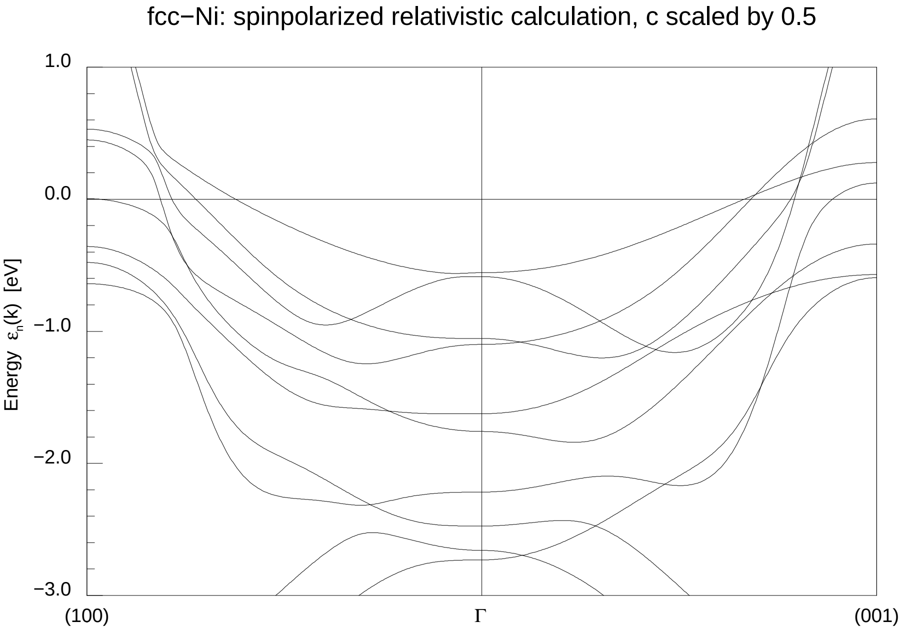

Figure 7: Band structure of ferromagnetic fcc-Ni. The velocity of light was scaled by a factor 0.5.

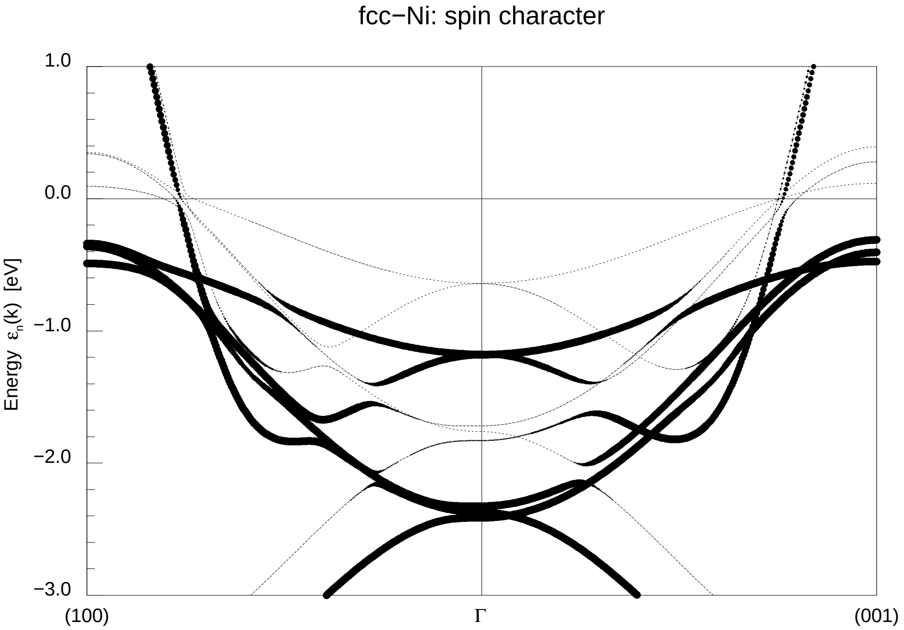

Figure 8: Band structure of ferromagnetic fcc-Ni with the spin character indicated by the size of the points. The largest size corresponds to pure majority spin character, while the smallest size corresponds to pure minority spin character.

Band structure of fcc-Ni: Lifting of degeneracies and spin characters

In the non-relativistic theory, the symmetry of the fcc-lattice implies degeneracies of the band structure at points of high symmetry like the Γ-point. Relativistic effects usually lead to a reduction of symmetry in ferromagnetic metals. As a consequence, the corresponding representations of all one atomic lattices become one-dimensional [14] and group theoretical arguments do no longer imply degeneracies of the band structure, with the remaining degeneracies being accidental. On an intuitive level this fact may be understood if one lets the lattice constant go to infinity: The symmetry is still the same, but the bands become flat with energies corresponding to the atomic levels, which are non-degenerate. As an example, a band structure of fcc-Ni is shown in Fig. 7. To emphasize the effect, the bands drawn are taken from a calculation with the velocity of light set to $c/2$.

Another effect implied by the relativistic theory is that the spin is no longer a good quantum number. Thus a simple splitting into spin up and spin down bands is not appropriate anymore. However, a projection onto spin states as demonstrated in Fig. 8 can be useful.

Equilibrium lattice constant of thorium

The evaluation of equilibrium lattice parameters is one of the fundamental goals of density functional calculations. It is, within a given approximation of the xc functional, a well-defined task and ideal for comparing the reliability of different numerical methods.

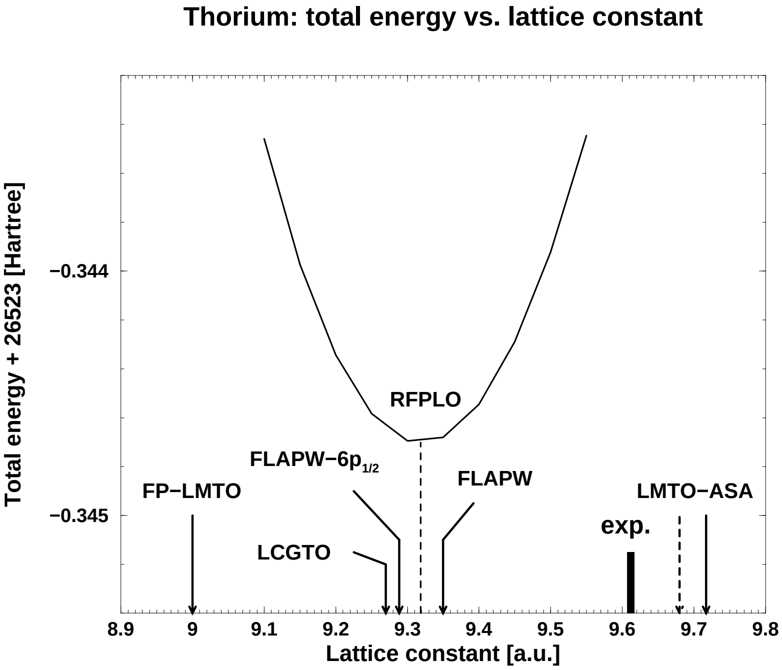

Figure 9: Equilibrium lattice constant of thorium: comparison of experimental data and LDA results obtained by different numerical schemes.

Figure 9 shows the dependence of the total energy of fcc thorium on the lattice constant obtained with RFPLO using the Perdew-Wang 92 LDA [15]. The position of the minimum is indicated by a dashed line. Further, the experimental lattice constant is given by a box, where the width shows the scatter of experimental data from Pearson's table. Equilibrium lattice constants obtained by five different methods are denoted by arrows: LMTO-ASA [16]; FP-LMTO [17];

LCGTO-FF and FLAPW [18]; FLAPW-6p$_{1/2}$ (unpublished data obtained as described in Ref. [19]).

The value obtained by LMTO-ASA refers to room temperature [16], but the related zero-temperature value (dashed line, estimated from the linear coefficient of thermal expansion) is not so much below the former one. At the first glance, one could be happy with LMTO-ASA, yielding a result quite close to (but above!) the experiment. If we turn to the full-potential version, FP-LMTO, that should provide a numerically more accurate result by definition, it becomes clear that ASA is not suited for a quantitative analysis of lattice geometries.[2] Note, that both calculations used the same version of LDA (Hedin-Lundqvist) and included spin-orbit coupling in the so-called second variational step [20]. The latter method suffers from convergence problems of the employed basis of spin eigenstates [21]. Careful convergence of this basis in an FLAPW calculation [18] yields a result about 2.5% below the experimental value, as commonly obtained in LDA. In the same publication, LCGTO-FF results were presented. This method uses an approximation for the full Dirac equation different from the second variational step. As pointed out in Ref. [18], both calculations should provide approximate upper and lower bounds, respectively, for the spin-orbit effects.

Going to still more accurate treatments of spin-orbit coupling, we indeed find results between the latter two. Local 6p$_{1/2}$-states were included in FLAPW recently [19], thus reducing the convergence problem of the spin eigenstate basis considerably (FLAPW-6p$_{1/2}$). Finally, the RFPLO result is given (curve and dashed line), were spin-orbit coupling is exactly treated in the limits of the Kohn-Sham-Dirac equation.

It is quite satisfactory that the results of the two most accurate methods are close to each other (though not yet as close as the different experiments) and between the bounds provided by LCGTO-FF and FLAPW. Such a level of reproducibility with completely different numerical methods can provide a save basis for the development of improved xc functionals.

FPLO-2

The latest version of the code, FPLO®-2, has been released recently.[3] Licenses for using the code are issued for a moderate fee. You can find the related conditions at the FPLO homepage, **http://www.ifw-dresden.de/FPLO/**. We distribute the release by email. It consists of source code in Fortran and C and a short documentation. The scalar relativistic version of FPLO is included in FPLO®-2, but not the fully relativistic one. In the course of the year 2002, we intend to distribute an update with the CPA and LSDA+U options, both included in the present license.

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[2] We would like to emphasize, however, that a number of important qualitative results has been obtained by this efficient method in the past.

[3] The release number 2 refers to the year 2002.

Portability

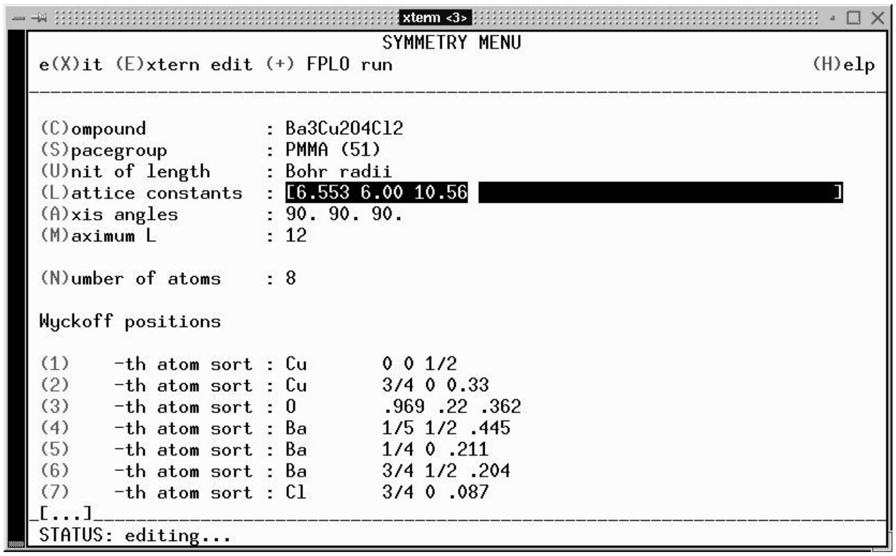
What is needed for installing and using FPLO®-2, is a UNIX-derived operating system with ANSI-conform C compiler and f90 compiler. We have tested the portability for the following platforms:

operating system	compiler
Linux	ifc
Linux	pgf90
IRIX	vendor f90
True64	vendor f90
AIX	vendor f90
HP-UX	vendor f90

Note, that we cannot guaranty the function on other platforms. In particular, other than the mentioned f90 compilers may yield reduced performance or do not suite at all. In any case, it is highly recommendable to use the most recent compiler release.

User interface

The user interface comprises not only the necessary tools to set up and modify the input files for running the code, but also several tools for presentation and processing the output data. Figure 10 shows a screen-shot of the specifically designed input-editor. It runs interactively with the main FPLO code, is operated by hot-keys and largely error-resistant. The example shown is $Ba_3Cu_2O_4Cl_2$, an anti-ferromagnetic compound out of the large family of the copper-oxides containing 22 atoms per elementary cell. More complicated elementary cells may consist of more than one hundred atoms.



```
                              SYMMETRY MENU
e(X)it (E)xtern edit (+) FPLO run                                       (H)elp
-------------------------------------------------------------------------------

(C)ompound           : Ba3Cu2O4Cl2
(S)pacegroup         : PMMA (51)
(U)nit of length     : Bohr radii
(L)attice constants  : [6.553 6.00 10.56                                  ]
(A)xis angles        : 90. 90. 90.
(M)aximum L          : 12

(N)umber of atoms    : 8

Wyckoff positions

(1)    -th atom sort : Cu       0 0 1/2
(2)    -th atom sort : Cu       3/4 0 0.33
(3)    -th atom sort : O        .969 .22 .362
(4)    -th atom sort : Ba       1/5 1/2 .445
(5)    -th atom sort : Ba       1/4 0 .211
(6)    -th atom sort : Ba       3/4 1/2 .204
(7)    -th atom sort : Cl       3/4 0 .087
_[...]_________________________________________________________________________
STATUS: editing...
```

Figure 10: Screen-shot of the FPLO input tool.

Understanding the geometrical structure of a compound is an important condition for understanding its bonding and, in succession, all other chemical and physical properties. For this aim, a related presentation tool is utterly useful. Figure 4 has been produced with this tool.

Other tools are available for the presentation of Fermi surfaces and band structures on symmetry lines, including weighted ('fat') bands, and for the supervision of the iteration process.

Benchmarks

There are two quantities that chiefly determine the computing time and the memory allocation: the number of atoms in the elementary cell, and the number of k-points.[4] We present two example benchmarks here, the dependence of computing time per iteration cycle and memory allocation on the number of k-points, and the memory allocation in dependence of the complexity of the elementary cell. More extended benchmark tests will be presented at the FPLO homepage

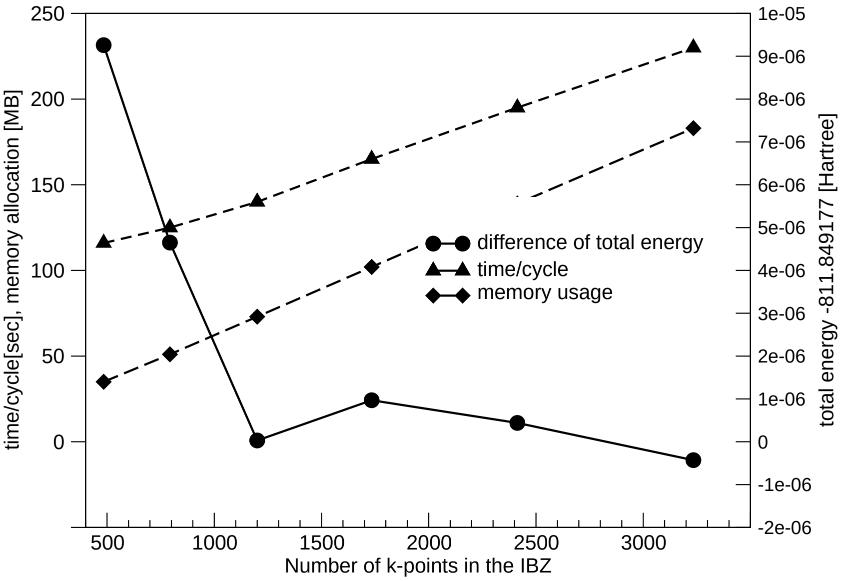


Figure 11: Example benchmark: ScB_2 with 3 atoms per unit cell, self consistent calculation with different numbers of k-points. Left axis: computing time per iteration cycle and memory allocation; right axis: total energy. The calculation was done on Origin3800, running IRIX6.5.

Figure 11 shows the dependence of computing time and memory allocation on the number of k-points in the irreducible part of the Brillouin zone for the example compound ScB_2 with 3 atoms per unit cell. As expected, both the computing time per iteration cycle and the memory allocation scale linearly with the number of k-points. There is a significant constant contribution to the computing time, i.e., choosing a large number of k-points does not significantly slow

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[4] In a strict sense, the number of k-points is of course determined by the accuracy requirements and cannot be chosen arbitrarily.

Table 1: Example benchmark: Memory allocation (on Origin3800, IRIX6.5) in dependence of the structure and number of k-points.

Compound	atoms/u.c.	k-points in IBZ	Memory [MB]
Al	1	72	6
Fe	1	72	9
ScB_2	3	191	63
$SrCoO_3$ cubic	5	35	27
$SrCoO_3$ orthorhombic	5	1331	555

down the calculation for small unit cells (up to about 10 atoms). Another important feature is that the total energy of the self consistent calculation is stable (for sufficiently large number of k-points) within 1 μHartree.

Some examples of the memory needed for different structures are compiled in Table 1. In cases were large numbers of k-points in the irreducible part of the Brillouin zone (IBZ) are needed the memory allocation is considerable already for unit cells of moderate size. We plan to implement a version with reduced memory demand in the forthcoming release.

Workshop "Hands-on-FPLO"

From March 3 to 7, 2002, IFW Dresden hosted the workshop "Hands-on-FPLO" that was supported by the ESF, STRUC-ψ_k. Purpose of the tutorial workshop was to provide an introduction into the concept, the code, and the handling of the FPLO package including the ability to cope with simple problems that may arise when using the code.

The workshop programme consisted of lectures held by the code developers and by experienced users of the code primarily in the morning hours, and exercises in the afternoon. While the first exercise was focussed on "getting started" (fcc-aluminum: how to create the input file, meaning and handling of the output), all participants were able to work on systems of their individual choice during the second and third day of the workshop. The number of participants (30 trainees from 9 different countries and 11 lecturers) was almost twice the originally planned number, demonstrating the need of fast and accurate DFT code. Twelve X-terminals, each connected to a separate dual node of our LINUX cluster, were available to the participants. In this way, the group size could be kept moderately small and (almost) individual work was possible.

As the main result of the workshop, all participants are able to handle the code for routine calculations. The participants further started calculations on systems of their choice. In cases were difficulties with the code handling encountered, they could be solved together with the tutors. Licenses to use the code for academic purposes were issued to the home departments of all participants (15 in total). The second workshop "Hands-on-FPLO" is scheduled for March, 2003.

Summary and Outlook

We finally summarize the features of the recently developed full-potential local-orbital minimum-basis (FPLO) scheme in brief.

- FPLO uses a locally finite lattice sum for the representation of the full potential by a partitioning of unity. This enables a treatment of the multi-center integrals both efficient and accurate.
- The algebraic dimension of the problem is reduced by a fast and exact elimination of the core states.
- FPLO uses a variable local orbital basis which is readjusted to the potential at each iteration step of self-consistency.
- During the iterations of self-consistency, the basis orbitals are simultaneously optimized by individual parameter variation to minimize the total energy.
- Given a density functional, FPLO has a thoroughly tested numerical accuracy of better than 2 mHartree per atom for the absolute value of the total energy.
- Up to about N=100 atoms per unit cell, FPLO performs approximately as $N^{1.5}$. It is extremely efficient with a large number of **k**-points, an important issue in applications to metals.
- There exist a fully 4-component relativistic version, a scalar relativistic version, and a flexible CPA implementation for substitutional alloys. Rotationally invariant LSDA+U is implemented as well.

As an outlook, we intend to release FPLO®-3, comprising the present release and the fully relativistic code, in 2003.

Acknowledgment

It is difficult to trace all contributions that have entered a development that, with varying intensity, took several decades. Most recently, the following colleagues contributed in various ways to the success of our project: Arthur Ernst, Helge Rosner, Michael Kuzmin, Roland Hayn, Arnulf Möbius, Vito Servedio, and Saad Elgazzar. Our Prague colleagues kindly helped us by doing careful comparison with the WIEN code: Martin Diviš, Pavel Novák, and Jan Kuneš.

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