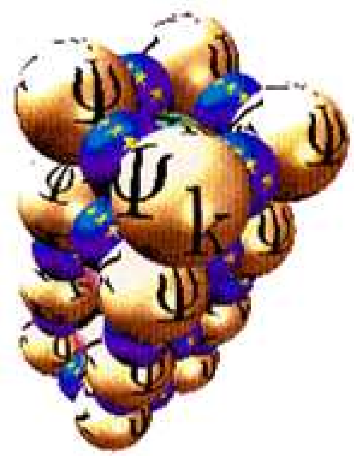
Ψ_k Newsletter

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

Number 75 June 2006



Editor: Z. (Dzidka) Szotek
E-mail: psik-coord@dl.ac.uk

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Contents

1 Editorial

This Psi-k Newsletter contains a number of reports on workshops which can be found in the RTN "f-Electrons" section and the ESF Psi-k Programme section. This time we also have one report on a collaborative visit in the latter section. Several announcements of future meetings/schools/workshops can be found in the ESF Psi-k Programme section and the section of the General Workshop/Conference Announcements. The available position announcements and abstracts of the newly submitted or recent papers are in their usual sections. In the section "Presenting Other Initiatives" we have some information on graduate courses. As usually, the newsletter is finished with a scientific highlight by Etienne Balan (*Aix en Provence* and *Paris*), Michele Lazzeri (*Paris*) and Francesco Mauri (*Paris*) on **"Infrared spectrum of hydrous minerals from first-principles calculations"**. Please check the table of contents of the newsletters 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 2006 workshops and hands-on courses (subject to funding).

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@dl.ac.uk	**messages to the coordinators, editor & newsletter**
psik-network@dl.ac.uk	**messages to the whole Ψ_k community**

Z. (Dzidka) Szotek, Martin Lüders and Walter Temmerman
e-mail: psik-coord@dl.ac.uk

2 News from the RTN on "f-electrons"

"Ab-initio Computation of Electronic Properties of f-electron Materials"

2.1 Reports on RTN2 Workshops

2.1.1 Report on Workshop on the "Physics of f-electron Solids"

1-2 April 2006, Canterbury, U.K.
Sponsored by
RTN2 "f-electrons" and UK's CCP9 Programme

On March 30th to April 2nd a group of twenty physicists met at a weekend workshop to discuss the most recent advances in the electronic structure of f-electrons. The meeting was held under the auspices of the University of Kent in the picturesque surroundings of the International Study Centre of Canterbury Cathedral which is within the precincts of the Cathedral itself. The workshop was organised within the framework of the RTN2 network 'Psi-k: f-electrons' by Walter Temmerman, Axel Svane and Paul Strange.

The meeting was opened with a talk from Misha Katsnelson (Nijmegen) who explained the latest developments in Dynamical Mean Field Theory (DMFT) and showed how the LDA-DMFT can be solved using a fluctuating exchange approximation and he then went on to explain how this method describes materials where strong correlations play a major role in determining the properties. The talk was illustrated with a series of applications, particularly to actinide chalcogenide materials. He also showed hoe the method yields insight into superconductivity in $PuCoGa_5$ and discussed the (non)magnetic states in δ-Pu. Aspects of DMFT implementations were discussed in subsequent talks by L. Poyourovskiy on actinide and rare-earth compounds, and by F. Lechermenn on the construction of appropriate Wannier functions for the optimum representation of many-body operators.

Ian Hughes from Warwick presented a talk on the application of the Disordered Local Moment approach to the magnetism of rare earth materials. The method is implemented using the KKR-CPA with Local Self-Interaction Corrections. This method was used to calculate the susceptibility inn HCP Gadolinium. Gadolinium is known experimentally to be ferromagnetic and this was reproduced by the calculation. They were also able to calculate thelattice constant and Curie Temperature in good agreement with experiment and to show that the ferromagnetic arrangement of spins wins out in competition with more exotic spiral structures characteristic of other rare earth elements. The results were discussed in detail in terms of nesting features in the Fermi surface.

Olle Eriksson (Uppsala) described the method of projector functions which are used in LDA+U or Self-interaction corrected electronic structure theories. These are constructed to reproduce the spin and orbital magnetic moment of the material for the atomic many body state. Once they have been calculated they can be used in conjunction with any electronic structure method to calculate ground state properties.

Helmut Eschrig (Dresden) discussed the background to the calculation of orbital moments in materials and discussed how to calculate them accurately for actinide materials. In relativistic density functional theory it is a four-current, rather than the density that is the basic quantity. This quantity couples to the electromagnetic field and can be described by the Kohn-Sham-Dirac equation in the usual way. If a non-relativistic limit of this theory is taken it yields a simple Zeeman effect which can be well-described within the LSDA, spin-orbit coupling and an orbital current. This latter coupling is what leads to Hund's second rule in atoms. This latter coupling has been described until recently by the empirical orbital polarisation term introduced by Eriksson and Brooks. In this talk Professor Eschrig described a derivation of an orbital polarisation xcorrection potential from the non-relativistic limit of the Kohn-Sham-Dirac equation which is valid in limited conditions. The derived expression is similar to the ad-hoc Eriksson-Brooks expression and was shown to give good values of the orbital polarisation in Heusler alloys.

Gerrit van der Laan gave a talk entitled "Probing the Population of the Spin-Orbit Split Levels in the Actinide 5*f* States" The spin-orbit interaction in the 5f states is key to understanding the exotic electronic and magnetic properties observed in actinide metals and compounds. He reported that the branching ratio of the white-line peaks of the N-4.5 edge for the light actinide metals, alpha-Th, alpha-U, and alpha-Pu were recorded using electron energy-loss spectroscopy in a transmission electron microscope X-ray absorption spectroscopy (XAS). He explained how to use the spin-orbit sum rule and the branching ratios from both experimental spectra and many-electron atomic spectral calculations, accurate values of the spin-orbit interaction, and thus determine the relative occupation of the j = 5/2 and 7/2 levels for the actinide 5f states. The results demonstrate that the spin-orbit sum rule works very well with both EELS and XAS spectra. This is important, since the high spatial resolution of a TEM can be used to overcome the problems of single-crystal growth often encountered with actinide metals, allowing acquisition of EELS spectra, and subsequent spin-orbit analysis, from nm-sized regions. For Pu it was shown that L-S coupling fails for the 5f states and that j-j coupling does not provide an accurate description either. It was shown that an intermediate scheme must be used for the actinides because of the considerable spin - orbit interaction in the 5f states.

Paul Strange (Kent) and Simon Brown (ESRF) described the state of the art in theory and experiment in describing resonant x-ray scattering from rare earth elements. Using a combination of x-ray polarisation and experimental geometry it is possible to turn off quadrupolar contribution to the scattering. The theory of x-ray scattering is described using 2nd order time-dependent perturbation theory. To calculate the spectroscopic cross section a good description of the electronic structure of the materials is required and this is provided by the LDA and density functional theory with self-interaction corrections. Cross sections and asymmetry ratios were calculated at the L3 edge for all the heavy rare earth metals. The experiments were carried out on the Xmas beamline at the ESRF and excellent agreement with the theory was found.

A two-peak structure in the asymmetry ratio was found. Analysis of the electronic structure provided an interpretation of the peaks in terms of scattering from the orbital and spin contribution to the magnetic moments. There is a large change in the asymmetry ratio as we proceed across the periodic table from Ho-Er-Tm. It was shown that this is due to scattering from the magnetic moments and that the changes are due to the magnetic moment changing from being spin-dominated to orbital dominated.

Sebastien Lebegue (Universite Henri-Poincare) described calculations using the Hubbard-1 approximation in which the embedding of an isolated f(n) ion in a solid is performed by modifying the crystal Hamiltonian as obtained from the local-density approximation with the atomic self-energy of the ion. The parameters of the model are obtained from the self-consistent band structure calculation. This method is then used to calculate the electronic structure of rare earth compounds including multiplet effects and these can be directly compared with experimental x-ray photoemission spectra good agreement is found and it is clear that the experiment exhibits the multiplet structure. The theory was used to describe a series of Tm chalcogenides which also show a divalent/trivalent valence transition.

Balazs Gyorffy (Bristol) reported on the first implementations of the KKR-NLCPA (Korringa-Kohn-Rostocker Non-Local Coherent Potential Approximation) which facilitates the considerations of ensembles with Short Range Order (SRO). The calculations were for BCC Cu-Zn and FCC CuPd alloys. An interesting new feature of such calculations is that they yield different Cu and Pd potentials for different nearest neighbour configurational environments. This shows that these potentials imply an inhomogeneous splitting of the core-levels and it was demonstrated that these core-level shifts can be observed in a photoemission (XPS) experiment.

Rene Windiks (Materials Design, Le Mans) discussed applications of rare earth materials. In particular he showed some of the deep colours that can be obtained using rare earth materials as dyes. For instance pure and alkali-doped cerium sesquisulfides form red to orange pigments that are used on the industrial scale in the coloration of plastics, and as paints and coatings. Oxides of praseodymium and neodymium, respectively, mixed with glass compositions allow the manufacturing of green and purple colored glass pieces. The colours are due to electronic excitations on the rare earth cation. Although these are qualitatively understood a theory that will predict the colours depending on chemical composition and crystal structure is very desirable to the industry. The talk described the strategy fro gaining a deep understanding of the optical properties of these materials which initially involve LDA+U calculations and recently some first attempts at a DMFT description.

The final talk of the meeting was by Axel Svane (Aarhus) who described his work using self-interaction corrected density functional theory to describe rare earth impurities in the semiconductors GaAs. He was able to model these materials using LDA-SIC in supercell calculations. This enables him to find the lowest energy state for the rare earth which turned out to be for it to sit on the Ga site in a 3+ valence configuration. The $3+ \rightarrow 2+$ f acceptor level is found above the theoretical conduction band edge in all cases and within the experimental gap only for Eu, Tm and Yb in GaAs and for Eu in GaN. It was found that the exchange coupling between the impurity and the states at the valence band maximum and conduction band minimum is insufficient to yield magnetic order in dilute impurities.

Programme: f-electron Workshop

09:00 -- 10:00	Misha Katsnelson: Correlation Effects in Actinide Compounds.
10:00 -- 10:30	Ian Hughes: Magnetic Ordering in the Rare Earths from Ab-initio.
10:30 -- 11:00	Coffee
11:00 -- 11:45	Sebastien Lebegues: Multiplet Effects in the Electronic Structure of Rare Earth Compounds.
11:45 -- 12:30	Helmut Eschrig: Orbital Polarisation Corrections to Magnetism.
12:30 -- 14:00	Lunch
14:00 -- 14:45	Olle Eriksson: On Hund's third rule and a description of atomic projector orbitals in first principles calculations.
14:45 -- 15:30	Gerrit van der Laan: Probing the Population of the Spin-Orbit Split Levels in the Actinide 5f States
15:30 -- 16:00	Coffee
16:30 -- 17:00	Paul Strange: Theory of Resonant X-Ray Scattering in the Heavy Rare Earths
17:00 -- 17:30	Simon Brown: Resonant X-Ray Scattering in the Heavy Rare Earths

Sunday:

08:30 -- 9:15	Balazs Gyorffy: NL-KKR-CPA and the disordered local moment picture.
09:15 -- 09:45	Rene Windiks : Optical Properties of Rare Earth Oxides and Sulfides: Beyond the Local Density Approximation.
09:45 -- 10:15	Leonid Poyurovskii: Spectral and Optical Properties of Correlated f-electron Compounds: LDA + DMFT Approach.
10:15 -- 10:45	Coffee

10:45 -- 11:15   Frank Lechermann: Recent Developments Concerning Wannier Functions in DMFT

11:15 -- 12:00   Axel Svane: Theory of Rare Earth Impurities in GaAs and GaN.

12:00   Close of meeting and lunch

List of Participants: f-electron Workshop

Amft Martin	Martin.Amft@fysik.uu.se
Bjorkmann Torbjorn	Torbjorn.Bjorkman@fysik.uu.se
Brown Simon	sbrown@esrf.fr
Eriksson Olle	Olle.Eriksson@fysik.uu.se
Eschrig Helmut	H.Eschrig@ifw-dresden.de
Gyorffy Balazs	B.Gyorffy@bristol.ac.uk
Hughes Ian	I.D.Hughes@warwick.ac.uk
Katsnelson Mikhail	M.Katsnelson@science.ru.nl
Lebegues Sebastien	Sebastien.Lebegue@lcm3b.uhp-nancy.fr
Lechermann Frank	Frank.Lechermann@cpht.polytechnique.fr
Lueders Martin	M.Lueders@dl.ac.uk
Pourovskii Leonid	Leonid.Pourovskii@cpht.polytechnique.fr
Strange Paul	P.Strange@kent.ac.uk
Svane Axel	Svane@phys.au.dk
Szotek Dzidka	Z.Szotek@dl.c.uk
Temmerman Walter	W.M.Temmerman@dl.ac.uk
Van der Laan Gerrit	G.van_der_laan@dl.ac.uk
Windiks Rene	Windiks@swissonline.ch
Zenia Hand	H.Zenia@sheffield.ac.uk

Abstracts

Correlation effects in actinide compounds

M. I. Katsnelson

Institute for Molecules and Materials, Radboud University of Nijmegen,
NL-6525 ED Nijmegen, The Netherlands

A review is done of our recent electronic structure calculations for $5f$ compounds [1–3] in the framework of LDA+DMFT (dynamical mean-field theory) scheme. To solve effective quantum impurity problem, we use a perturbative approach based on the fluctuating exchange (FLEX) approximation with taking into account T-matrix renormalization of the bare Coulomb interaction (SPTF approach [1, 4]). This approximation works with complete four-index interaction matrix and take into account arbitrarily strong spin-orbit interaction. We focus on the discussion of magnetic properties of actinide compounds. The method was tested for actinide monochalcogenides (USe, UTe, PuSe, and PuTe) and results in a good agreement with experimental data for both magnetic properties and photoemission spectra. We have calculated also electronic structure of $PuCoGa_5$ and UGe_2; in the first compound an extended Van Hove singularity near the Fermi energy is found which can play an important role in its superconductivity. We discuss also a controversial problem of nonmagnetic strongly correlated state for δ-Pu.

References

[1] L. V. Pourovskii, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B **72**, 115106 (2005).

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[3] L. V. Pourovskii, M. I. Katsnelson, A. I. Lichtenstein, L. Havela, T. Gouder, F. Wastin, A. B. Shick, V. Drchal, and G. H. Lander, to appear in Europhys. Lett.

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Magnetic Ordering in the Rare Earths from *ab-initio*

I. Hughes[1], M. Däne[2], A. Ernst[3], W. Hergert[2], M. Lüders[4], J. Poulter[5],
J.B. Staunton[1], Z. Szotek[4] and W.M. Temmerman[4].

[1]Department of Physics, University of Warwick, U.K.
[2]Fachbereich Physik, Martin-Luther-Universität, Halle-Wittenberg, Germany.
[3]Max Planck Institut für Mikrostrukturphysik, Halle, Germany.
[4]Daresbury Laboratory, Warrington, U.K. [5]Mahidol University, Bangkok, Thailand.

We investigate the onset of magnetic order in rare-earth systems using a ‘first-principles’ theory of metallic magnetism, in which strong electron correlations are included. Thermally induced spin fluctuations are treated within a mean-field ‘disordered local moment’ (DLM) picture [1] and the scheme is implementated using a Korringa Kohn Rostoker-coherent potential approximation (KKR-CPA) method [2]. The recently developed local self-interaction correction (L-SIC) method of Lüders *et al* [3] is used to incorporate strong electron correlation effects.

We apply the theory to hcp-gadolinium. Within standard electronic structure methods, based on the local spin-density approximation (LSDA), this system is predicted to have an antiferromagnetic groundstate [4], whereas experimentally it is ferromagnetic. Our method produces the correct magnetic groundstate for both the experimental and theoretical lattice parameters, as well as a good estimate of the Curie temperature. We observe that the ferromagnetic ordering is competition with a more complicated helical incommensurate ordering. It is shown that the relative strengths of the two ordering types depends strongly on the lattice parameters. The results are discussed in terms of changes to the fermi-surface in the disordered paramagnetic phase. We also present results for γ-Ce.

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[1] J. Hubbard, Phys. Rev. B **19**, 2626 (1979).

[2] B.L. Gyorffy *et al.*, J. Phys. F **15**, 1337 (1985); J.B. Staunton *et al.*, J. Phys. F **15**, 1387 (1985).

[3] M. Lüders *et al.*, Phys. Rev. B **71**, 205109 (2005).

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Multiplet Effects in the Electronic Structure of Rare Earth Compounds

Sebastien Lebegue

Laboratoire de Cristallographie et Modelisation des Materiaux
Mineraux et Biologiques (LCM^{3}B, UMR-CNRS 7036), Universit Henri Poincare, Nancy, France

The spectral functions of several rare earth compounds are presented including multiplet effects, and compared to experimental x-ray photoemission spectra. The basic tool is a Hubbard-I description of an isolated f^n ion, the Green's function of which is embedded in a solid state Hamiltonian as obtained from the local-density-approximation. The parameters of the model are calculated from the self-consistent bandstructure calculation. The agreement with experiment is excellent reproducing all significant multiplet structures.

Orbital Polarization in Density Functional Theory

Helmut Eschrig
IFW Dresden, P.O.Box 27 00 16, D-01171 Dresden, Germany
(with M. Sargolzaei, K. Koepernik and M. Richter)

In a relativistic approach, magnetic fields (externally applied or caused by spontaneous polarization) couple to the electron system via the minimal coupling to the four-current. Nonrelativistically, there is the Zeeman coupling to the spin density, accounted for in the Local

Spin-Density Approximation (LSDA) of Density Functional Theory (DFT), the indirect coupling to the orbitals via lowest order spin-orbit coupling (SO), and a direct coupling to orbital current via the vector potential, an orbital polarization (OP) term leading for instance to Hund's second rule in atoms.

The first two of these couplings are accounted for in many DFT calculations of magnetic systems within LSDA plus a second variational step for SO or by solving the Kohn-Sham-Dirac equation (KSD) in LSDA. For the third coupling until recently there was only an *ad hoc* OP correction term introduced by Eriksson and Brooks [1] (which in many cases gives quite reasonable corrections to orbital moments of magnetic materials). Besides, there exist variants of a non-relativistic current-density functional theory, which however are adjusted to the polarized homogeneous electron system and do not take into account the particular situation of an unfilled inner nearly localized atomic shell.

In a recent paper [2], an attempt was made to systematically derive such an OP correction potential from the KSD equation in the non-relativistic limit. Unfortunately, the program can only incompletely be carried through as there are reasonable but uncontrolled approximations to be made in two steps of the derivation. Nevertheless, the result is quite close to the *ad hoc* ansatz.

The derivation is sketched and examples of application are given. Among them, the influence of orbital polarization on half-metallicity of Heusler alloys is presented.

[1] O. Eriksson, M.S.S. Brooks and B. Johansson, Phys. Rev. B **41** (1990) R7311.

[2] H. Eschrig, M. Sargolzaei, K. Koepernik, M. Richter, Europhysics Letters **72** (2005) 611.

Many-body projector orbitals for electronic structure theory of strongly correlated electrons

O. Eriksson
Department of Physics, Uppsala University, Box 530, 751 21 Uppsala, Sweden

We describe a technique to evaluate projector functions to be used e.g. in self-interaction corrected versions of the Kohn-Sham equation (or in the LSDA+U method). The projector functions reproduce by construction the expectation values of spin and orbital moments (or any other property one is interested in) for the atomic many-body state. We therefore refer to these projector functions as many body projector orbitals (MBPO). It is described how, once these projector states have been calculated, one can use them in any electronic structure method for a solid or molecule, to calculate ground state properties of materials with strongly correlated states.

Probing the Population of the Spin-Orbit Split Levels in the Actinide $5f$ States

G. van der Laan
Magnetic Spectroscopy, Daresbury Laboratory, Warrington WA4 4AD, UK

The branching ratio of core-valence transitions in electron energy-loss spectroscopy and x-ray absorption spectroscopy is linearly related to the expectation value of the spin-orbit operator of the valence states. Here, we analyze the branching ratio of the $N_{4,5}$ edges in the actinides and find that the spin-orbit sum rule gives an accurate result without the need to include the core-valence interactions. The branching ratio is not only useful to study the variations in the $5f$ spin-orbit interaction, it also allows us to constrain the $5f$ count for given angular-momentum coupling conditions.

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Resonant X-Ray Scattering at the L3 edge of the rare earth metals

Paul Strange,

School of Physical Sciences, University of Kent, CT2 7NH

This talk is half of a joint presentation with Dr Simon Brown (ESRF). We will discuss a systematic combined experimental and first principles theoretical investigation of the resonant x-ray scattering at the L3 edge of the heavy rare earth metals. The theory is based on a first principles self-interaction corrected density functional theory description of the electronic structure of the materials and the spectroscopic quantities are found from standard second order time-dependent perturbation theory. In the talk I will outline the theory and compare it directly with experiment. Good qualitative agreement is observed and discussed.

Resonant X-Ray Scattering at the L3 edge of the rare earth metals; II

Simon Brown

XMaS, ESRF, 6 Rue Jules Horowitz F - 38043 Grenoble Cedex France

This talk is half of a joint presentation with Prof. Paul Strange (University of Kent). We will discuss a systematic combined experimental and first principles theoretical investigation of the resonant x-ray scattering at the L3 edge of the heavy rare earth metals. The experimental investigations were carried out on the XMaS UK CRG beamline at ESRF, employing both XRMS from antiferromagnetic phases and magnetic-charge resonant interference scattering from ferri/ferromagnetic phases. I will present the experimental results in conjunction with the first principles calculation. This approach has allowed identification of pre-edge dipolar excitations throughout the heavy rare-earth series. I will also present a model allowing separation of spin and orbital contributions to the observed/calculated spectra, which demonstrates a clear crossover from spin to orbital dominated magnetism either side of erbium in the lanthanide row.

The Non-Local Coherent Potential Approximation (NLCPA) and the generalized Disordered Local Moment Picture (DLM)

Balazs L. Gyorffy

H.H.Wills Physics Laboratory, University of Bristol Tynadall Ave. Bristol, BS8 1TL

Collaborators: D.Rowlands, A. Ernst, M.Lueders, W.Temmerman and Z. Szotek

A way to describe fluctuations about the Local density Approximation (LDA) in the Density Functional Theory for electrons in condensed matter is to constrain the local charge density and magnetization density and average over an ensemble of such constraints using the KKR-CPA. This is the conventional and very successful DLM picture. In this talk I will report on the first implementations of the KKR-NLCPA which facilitates the considerations of ensembles with Short Range Order (SRO).The calculations are for BCC Cu-Zn and FCC CuPd alloys .An interesting new feature of such calculations is that they yield different Cu and Pd potentials for different nearest neighbour configurational environments. I will show that these potentials imply an inhomogeneous splitting of the core-levels and that these core-level shifts can be observed in a photoemission (XPS) experiment. Furthermore, I will discuss the significance of observing the corresponding shifts in systems described by the DLM picture.

Optical Properties of Rare Earth Oxides and Sulfides: Beyond the Local Density Approximation

Rene Windiks

Materials Design s.a.r.l., 44, avenue F.-A. Bartholdi, 72000 Le Mans, France

There are a plenty of materials whose optical properties are determined by rare earth (RE) cations. For instance, pure and alkali-doped cerium sesquisulfides are nontoxic inorganic pigments of red to orange hue which are used on the industrial scale in the coloration of plastics, as paints and coatings.[1] Oxides of praseodymium and neodymium, respectively, mixed with glass compositions allow the manufacturing of green and purple colored glass pieces.[2] The chromatic properties of both classes of materials are due to electronic excitations in the range of 1.7–2.8 eV, the visible spectrum of radiation. Optical measurements as well as earlier calculations within the local density approximation provided a qualitative insight into the electronic structure of these compounds and pointed to the importance of f-electrons in the optical transitions. However, these earlier calculations were too blunt and did not provide quantitative predictions of optical gaps.[2,3] Systematic modifications and the design of novel compounds would greatly benefit from a detailed understanding of the relationships between the chemical composition, the crystallographic structure, and the optical properties. The main goals of the present effort are a clearer understanding of the absorption mechanism and quantitative predictions of the optical absorption in this class of compounds. Since elements with f-electrons belong to the class of strongly correlated systems, density functional methods extended with a Hubbard-U term (DFT+U) as well as approaches within the dynamical mean-field theory (DMFT) seem to be the theoretical techniques of choice. We present detailed DFT+U calculations and first steps towards a DMFT treatment. We discuss the role of the f-electrons in the optical transitions offering better quantitative predictions.

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Spectral and optical properties of correlated f-electron compounds: LDA+DMFT approach

Leonid Poyurovskiy.

cole Polytechnique - CPHT, F91128 Palaiseau Cedex, France

We have investigated spectral and optical properties of a number of 4-f and 5-f correlated materials using the LDA+DMFT technique. A perturbative spin-polarized spin-orbit T-matrix and fluctuating exchange (SPTF+SO) approach has been employed as a DMFT quantum impurity solver in order to treat moderately correlated metallic actinide compounds. The theoretical spectra of Pu and U monochalcogenides reproduces many-body features (the quasiparticle peak in vicinity of the Fermi energy, as well as smaller features at lower energies) of experimental photoemission. The LDA+DMFT calculations predict paramagnetic ground state for these compounds in agreement with the experiment. In ferromagnetic superconductor UGe_2 the LDA+DMFT calculations are able to reproduce features observed in angular resolved photoemission (ARPES) experiments. For the rare-earth sesquioxides La_2O_3 (La=Ce, Pr, Nd, Pm), which are Mott insulators, we have employed the Hubbard-I quantum impurity solver as well as full selfconsistency over charge density in the LDA+DMFT calculations. The experimentally observed tendency of increasing the band gap along the light rare earth sesquioxide seria is correctly reproduced. The band gap is between the lower Hubbard band and the unoccupied rare earth $d-$band in Ce_2O_3 and Pr_2O_3, while in the later sesquioxides one finds the oxygen $p-$band at the top of the valence band and the upper Hubbard band at the bottom of the conduction band. The LDA+DMFT optical conductance of the sesquioxides have been evaluated and it is in good agreement with experimental measurements.

Recent Developments concerning Wannier Functions in DMFT

Frank Lechermann

Centre de Physique Théorique, École Polytechnique

Palaiseau, France

An understanding of the physics of strongly correlated multi-orbital electron systems is one of the key ingredients in order to describe a wide range of novel solid state compounds. The complex interplay of the crystal structure with the competition between the localized and the itinerant character of electrons in a manifestly multi-orbital case is giving rise to highly interesting physical phenomena.

By combining the Dynamical Mean Field Theory (DMFT) with the Local Density Approximation (LDA) to Density Functional Theory, a powerful many-body approach is provided to tackle the given problem on a realistic level. This unified approach is naturally formulated by introducing Wannier functions as the basis representation for the electronic structure problem. The choice of Wannier functions is not unique in various senses and has to be tailored to the physical problem of interest as well as to the utilized theoretical framework.

We will discuss recent developments in this important area of interfacing realistic band-structure methods with DMFT by presenting results of current investigations of transition-metal oxides and sulfides.

Electronic structure of rare-earth impurities in GaAs and GaN

Axel Svane

Department of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark

The electronic structures of substitutional rare-earth (RE) impurities in GaAs and cubic GaN are calculated. The total energy is evaluated with the self-interaction corrected local-spin density approximation, by which several configurations of the open 4f shell of the rare-earth ion may be investigated. The defects are modelled by supercells of type $\mathrm{REGa}_{n-1}\mathrm{As}_n$, for $n = 4$, 8 and 16. The preferred defect is the rare-earth substituting Ga, for which case the rare-earth valency in intrinsic material is found to be three in all cases. The $3+ \rightarrow 2+$ f acceptor level is found above the theoretical conduction band edge in all cases and within the experimental gap only for Eu, Tm and Yb in GaAs and for Eu in GaN. Approximate ways of obtaining f-removal energies are discussed. The exchange interaction of the rare-earth impurity with the states at both the valence band maximum and the conduction band minimum is weak, one to two orders of magnitude smaller than that of Mn impurities. Hence the coupling strength is insufficient to allow for ferromagnetic ordering of dilute impurities, except at very low temperatures.

3 News from the ESF Psi-k Programme

”Towards Atomistic Materials Design”

3.1 Reports on Collaborative Visits

3.1.1 Report on a Collaborative Visit of C. Melis (King’s College London), to M. Parrinello’s Group (ETH Zurich)

26th February - 11th March 2006

I recently visited Prof. Michele Parrinello’s group at ETH Zurich. The goal of my visit was to learn metadynamics, a technique recently developed by Prof. Parrinello’s group to explore free energy surfaces of complex polyatomic systems [1]. In particular, I am interested in evaluating the applicability of metadynamics to a particular biological problem: the activation of the 5-HT$_3$ neuroreceptor.

The 5-HT$_3$ receptor is a ligand-gated ion channel: when activated, it acts as a channel for ions from the outside to the inside of the cell. The activation is initiated by the binding with serotonin, 5-HT$_3$ neurotransmitter, which triggers a series of conformational changes culminating with the opening (gating) of the channel. Up to now, we have assessed the effects of mutating specific amino-acids in the binding site on the binding of serotonin to the 5HT$_3$ receptor, using density functional theory calculations, to elucidate mutagenesis experimental data.

Very recently a new gating mechanism for 5-HT$_3$ has been proposed [2]: a specific proline amino acid, in a specific loop in the receptor, is thought to isomerize from its trans to its cis conformation, acting as a switch for the opening of the channel. We want to complement these experiments with a theoretical investigation on the proline isomerisation in the loop. Since the isomerisation process has a fairly high energy barrier (20 kcal/mol in vacuum), we need to use an appropriate simulation technique: the metadynamics method seems an ideal technique for the problem we wish to address.

During my visit I first got familiar with the metadynamics technique by applying it to various small model systems. I then performed some preliminary calculations on the whole loop including the proline amino acid. The results were promising, confirming that metadynamics is a suitable method for the description of our problem.

The visit has been very useful to learn the metadynamics technique and to assess its suitability for studying the 5HT$_3$ gating process. I am grateful to the network for its financial support.

(Claudio Melis)

References

[1] A. Laio and M. Parrinello, Proc. Nat. Acad. Sci. **99**, 12562 (2002).

[2] S. C. R. Lummis, D. L. Beene, L. W. Lee, H. A. Lester, R. W. Broadhurst and D. A. Dougherty, Nature **438**, 248 (2005).

3.2 ESF Psi-k Programme Workshop/Conference Reports

3.2.1 Report on the International Workshop on "Ab initio Description of Iron and Steel Status and Future Challenges"

Science Meeting	:	Workshop
Identification Code	:	ADIS2006
Location	:	Ringberg Castle, Germany
Dates	:	19/02/2006 – 24/02/2006
Organizers	:	Dept. of Computational Materials Design Max-Planck-Institut für Eisenforschung Düsseldorf, Germany
Sponsors	:	Psi-k network in the framework of the ESF

Summary

The aim of this workshop hase been to provide a forum where internationally leading experts from different scientific communities (basic research, applied science, industry) may gather, present tutorial-like lectures on their methods, exchange the latest results, and identify future trends and developments. After each talk, there were lively and fruitful discussions about the suggested methods, final results, and future directions. The lively atmosphere and the tutorial character of the talks encouraged the participants to contribute to this exchange of ideas. Several contributed talks as well as a poster session gave all particitants the opportunity to discuss their latest results.

The scientific topic of the meeting, the ab initio based description of materials properties and processes, is a field of rapidly growing interest. The talks discussed various combinations of accurate quantum-mechanical description at the atomic scale with meso- and/or macroscale approaches such as thermodynamics, kinetics and phase field simulations and showed that this approach provides a qualitatively new level of predictive power. Examples, which have been successfully tackled by this approach ranged from fundamental aspects, e.g. science in the earth core, to industrial research activities in designing novel materials for engine blocks. The talks made also clear that despite recent tremendous success, these methods are still in their infancy and many open problems remain. Main challenges which have been discussed are the quest for an improved description on the atomistic level to obtain accurate ground states and potential energy surfaces, construction of efficient and accurate tools to map the first-principles results onto Ising-like Hamiltonians, incorporation of vibrational and anharmonic entropy contributions or accurate description of magnetism and its temperature-dependent effects. The participants of the workshop felt that to address these challenges a joint effort of the scientific groups working in the fields of ab-initio calculations and thermodynamic / kinetic modeling of materials is needed and that the ADIS2006 workshop served as an important step in this direction.

Description of the scientific content

The main contributions to the international workshop ADIS2006 were the tutorial-like lectures of the invited speakers. The large number (15) of these talks allowed a detailed overview of a broad scope of state-of-the-art simulation techniques for the description of iron, steel and related materials. The longer than usual talks (75min+15min discussion) allowed the speakers to give a profound insight into the fundamentals, the applicability and the outcome of specific ab-initio methods, and were the basis for very lively discussions. In the following a brief summary of the lectures:

Dario Alfè started the course with his concepts for a calculation of Gibbs free energies of iron from first principles. He performs density functional theory in conjunction with the technique of thermodynamic integration. Different approaches to melting, based on free energies and the coexistence method, were discussed. The theory was applied to the melting conditions of iron under Earth?s core conditions.

Frank Lechermann considered in his talk the ternary system Ni-Fe-Al as a test case for how far one can come with the calculation of finite-temperature phase diagrams of multi-component systems by a combination of the ab initio electron theory with statistical mechanics. For the calculation of the whole Gibbs triangle a mixed basis pseudopotential code was combined with the cluster-expansion method. Lechermann discussed the cluster-variation method of statistical mechanics in order to calculate the ab initio phase diagrams at finite temperatures.

Mojmír Šob focused in a first part on magnetic behavior changes of solids when a high-strain deformation is applied. He displayed total energies in contour plots as functions of distortions and volume, calculated by spin-polarized full-potential LAPW method. In a second part he briefly outlined the CALPHAD method for the construction of phase diagrams in alloys containing complex intermetallic phases. ?ob showed ab initio total energy differences (lattice stabilities) for sigma phase in Fe-Cr, Fe-Cr-Ni and Fe-Cr-Mo systems.

Gerbrand Ceder also pointed out that within the last fifteen years the cluster expansion technique has become a practical solution to predict the most stable structures and phase diagrams on a chosen parent lattice. By data mining more than 15,000 first principles energy calculations more than 85 alloys, he furthermore showed that the energies of different crystal structures are strongly correlated between different chemical systems, and demonstrated how this correlation can be used to boost phase stability investigations of new systems.

Mark Asta discussed applications of atomic-scale molecular-dynamics (MD) computer simulations to the calculation of interfacial thermodynamic and kinetic properties of both molecularly rough and faceted crystal-melt interfaces. A large range of aspects was mentioned, including the capillary fluctuation method, dendrite growth and structure selection in crystal nucleation from the melt, thermodynamic properties of steps on faceted crystal-melt interfaces and their mobilities. Animated examples for Fe, Mg, Si as well as other materials were shown.

Stefan Müller considered ab initio concepts for alloy properties, which possess a delicate temperature-dependence like short-range order or precipitate evolution. For this purpose he used the combination of DFT calculations with methods from statistical physics, namely Cluster Expansions (CE) and (Kinetic-) Monte-Carlo (MC) simulations. The mixed-space presentation for the treatment of long-range interactions and a new surface cluster-expansion allowing for an efficient selection and reduction of relevant interactions was explained.

Andrei V. Ruban presented his calculations of effective interactions in bcc Fe-Cr and fcc Fe-Cr-Ni alloys for different alloy compositions. He used the screened generalized perturbation method (SGPM) in conjunction with the KKR-ASA-CPA method. It was shown that magnetism plays crucial role in the ordering behavior of these alloys. Interactions were consequently used in the MC simulations of the atomic ordering effects and the results were compared with experimental data.

Peter Entel used first-principles calculations in order to obtain microscopic information of structural instabilities in transition metal compounds and alloys. These calculations allow to characterize martensitic trends associated with anharmonicities and phonon softening, magnetic ordering, electronic and chemical features. At finite temperatures, simulation of reactions of solids, thin films and nanoparticles were presented with the help of optimized interatomic potentials.

Pavel Korzhavyi presented various examples of theoretically derived composition-structure-property relations for several industrially relevant alloy phases, which include Fe-Ni-Cr austenite phase, oxi-carbo-nitrides of titanium, and iron-based sigma phases. He showed that ab initio calculations have reached the level at which they can provide quantitatively accurate description of the energetics of these phases as a function of their structure, composition, atomic and magnetic order and can be used for the CALPHAD approach.

Helmut Eschrig pointed out that the phase equilibrium under external fields (as stress or electromagnetic one) is preferably described by the Free Enthalpy, whereas the Free Energy is more easily obtained from total energy calculations. The interrelations between both were analyzed beyond linear response, and examples were discussed. Besides general elasticity, this included epitaxial paths as well as a fixed magnetic moment approach for invar and magnetostriction.

François Willaime studied from first principles defects and defect clusters in iron. He presented the methodological issues of calculations based on the SIESTA code, which changed in particular the energetic landscape of interstitial-type defects, as compared to what was known before from empirical potentials. The results were used as input data for the simulation of the kinetic evolution of radiation induced defects. This multi-scale approach allows reaching macroscopic time and length scales. The validity of empirical potentials was improved by including ab initio results in the database of fitted properties.

Matt Probert introduced a novel genetic algorithm for atomistic structure determination. It has been implemented in the ab initio DFT code CASTEP, where it can be used for the prediction of crystal structures from first principles, and in a simple pair potential code for algorithm development and testing. Results from both codes were presented, showing how the algorithm performs for a number of difficult problems, and how to best choose the various controlling parameters for optimal performance.

Peter E. Blöchl 's talk was devoted to the growth of atomically perfect, epitaxial oxide films on semiconductors as done using molecular beam epitaxy. In order to guide experiment he performed ab initio calculations using ab initio molecular dynamics and the projector augmented wave method. He investigated and discussed the atomic processes leading to perfect interfaces of semiconductors with high-K oxides.

Britta Nestler presented a recently developed non-isothermal phase-field model for alloys with multiple components and phases. The model has been derived from an entropy functional in a thermodynamically consistent way and allows to model arbitrary phase diagrams. She showed solidification microstructures on different time and length scales leading to the formation of dendritic and eutectic grain structures and the subsequent process of grain growth.

Christopher Wolverton described the role of atomic-scale first-principles computations in the Integrated Computational Materials Science methodology applied to Al castings at Ford. He focused on coupling first-principles methods with other computational approaches such as phase-field microstructural evolution models, computational thermodynamics or CALPHAD methods, cluster expansion methods and kinetic Monte Carlo. Applications were shown to prediction of precipitation, microstructure evolution, and ultimately yield strength during heat treatment.

Since all participants are currently doing research in the field defined by the scope of the workshop, there were extensive discussions after each lecture. Experienced researchers had ample time to debate different approaches. Junior researchers had plenty of opportunities to improve their understanding with specific questions.

In addition to the tutorial-like lectures several participants presented results of their research in 30minute talks and a poster session. These parts of the workshop were also characterized by vivid discussions and exchanges of ideas. In particular junior researchers had a chance to get a feedback of their research.

Impact of the event

A main achievement of the workshop ADIS2006 was to provide a platform for bringing together distinguished experts in ab-initio calculations and thermodynamic/kinetic modeling of metals and to provide an opportunity for exchange of knowledge and for fruitful scientific discussions. In the following a few highlights of the conference:

- There was consensus that the computational methods of density functional theory (DFT) have now reached the level at which they can provide a quantitatively accurate description of the energetics of metals and metallic alloy phases as a function of their atomic and magnetic order, composition and (defect) structure.

- For the simulation of binary and ternary alloys two classes of highly successful approaches have been discussed: The screened generalized perturbation method (SGPM) in conjunction with the KKR-ASA-CPA and the cluster expansion technique.
- The participants agreed that the current challenge of ab initio calculations is an extension towards the description of finite temperatures. A variety of approaches, including statistical mechanics, kinetic Monte Carlo and molecular dynamics, have been suggested and discussed at the workshop. Some participants reported that these approaches are already in a stage that they are relevant for industrial materials design. Nevertheless, a joint effort is still necessary to improve and validate these methods.
- Several participants have voted for a collection of electronic data obtained with ab initio calculations for various compounds and alloys. Such data bases would be a valuable complement to existing empirical data used for CALPHAD.
- Many participants that worked in different communities did not know each other before they came to Ringberg. Contacts have been established and people agreed to stay in contact after the workshop.

We, the organizers of the workshop, received a very positive feedback from the participants. There was a strong wish to repeat this meeting regularly (every two years) in order to exchange the latest results, and identify new trends and developments. We like to thank the Psi-k network in the framework of the ESF for financial support of the workshop ADIS2006.

Programme

Monday, February 20 (Ab initio Thermodynamics)

9:00 - 10:30	**Dario Alfè** (University College London, UK): *Thermodynamics of iron at high pressure and temperature from first principles calculations*
10:45 - 12:15	**Frank Lechermann** (École Polytechnique, France): *Ab initio thermodynamics for alloys: The ternary system Ni-Fe-Al as test case*
14:30 - 16:00	**Mojmír Šob** (Masaryk University in Brno, Czech Republic): *Ab initio studies of iron magnetism at high shape and volume deformations and predictions of structure of superaustenitic steels*
16:30 - 18:00	**Gerbrand Ceder** (MIT, USA): *New approaches to the ab initio prediction of phases diagrams and crystal structure in metals and alloys*
20:00 - 21:30	**Mark Asta** (University of California, USA): *Atomic-scale simulations of crystal-melt interface properties for multiscale modeling of solidification microstructure*

Tuesday, February 21 (Applications)

9:00 - 10:30	**Stefan Müller** (University Erlangen-Nürnberg, Germany): *Density functional theory meets statistical physics: From the local atomic structure to the mesoscopic properties of metal alloys*
10:45 - 12:15	**Andrei V. Ruban** (Royal Institute of Technology, Sweden): *Magnetism, effective interactions and atomic ordering effects in steels*
14:30 - 16:00	**Peter Entel** (University Duisburg-Essen, Germany): *First-principles investigations of structural transformations in magnetic solids, thin films and nanoparticles*
16:30 - 18:00	**Pavel Korzhavyi** (Royal Institute of Technology, Sweden): *Theoretical design of hard materials*
20:00 - 20:30	**Blazej Grabowski** (MPIE Düsseldorf, Germany): *Ab initio calculation of thermo dynamic properties of metals: xc-related error bars and chemical trends*
20:30 - 21:00	**Hans L. Skriver** (Technical University of Denmark): *Stability of nitrided stainless steel*
21:00 - 21:30	**Martin Friak** (MPIE Düsseldorf, Germany): *Anomalous equilibrium volume change of magnetic Fe-Al crystals*

Wednesday, February 22 (Fundamentals)

9:00 - 10:30	**Helmut Eschrig** (IFW Dresden, Germany): *General theory of phases of single crystals under stress*
10:45 - 12:15	**François Willaime** (CEA/Saclay, France): *Defects in iron from first principles: structure, stability and mobility*
13:15 - 18:30	**Excursion:** Technical Museum Munich

Thursday, February 23 (Methods and Surfaces)

9:00 - 10:30	**Matt Probert** (University of York, UK): *A novel genetic algorithm for atomistic structure determination*
10:45 - 12:15	**Peter Blöchl** (Clausthal Technical University, Germany): *Towards computational materials design of oxide films*
17:00 - 17:30	**Adam Kiejna** (University of Wroclaw, Poland): *First principles study of oxygen adsorption on iron surfaces*
17:30 - 18:00	**Duc Nguyen-Manh** (UKAEA Abingdon, UK): *Nano-clustering and impurity-defect interaction in Fe-Cr alloys: an ab initio study*
18:00 - 18:30	**Liverios Lymperakis** (MPIE Düsseldorf, Germany): *Ab initio based multiscale calculations of extended defects in condensed matter*
18:30 - 19:00	**Sergey Ostanin** (University of Warwick, UK): *Ab initio study of the soft-magnetic properties of permalloys*
21:00	**Poster Session**

Friday, February 24 (Towards Meso-/Macroscale)

9:00 - 10:30	**Britta Nestler** (Karlsruhe University, Germany): *A thermodynamically consistent phase-field model for alloys with multiple components and phases*
10:45 - 12:15	**Christopher Wolverton** (Ford Research Laboratory, USA): *What can we learn about precipitation in Al from first-principles?*

List of participants:

Hazem Abu-Farsakh (Max-Planck-Institut für Eisenforschung GmbH)
Dario Alfé (University College London)
Mark Asta (Northwestern University)
Ulrich Biedermann (Max-Planck-Institut für Eisenforschung GmbH)
Peter Blöchl (Clausthal University of Technology)
Alexander Blumenau (Max-Planck-Institut für Eisenforschung GmbH)
Sixten Boeck (Max-Planck-Institut für Eisenforschung GmbH)
Gerbrand Ceder (Massachusetts Institute of Technology)
Alexey Dick (Max-Planck-Institut für Eisenforschung GmbH)
Bernhard Eck (RWTH Aachen)
Peter Entel (Duisburg Campus)
Helmut Eschrig (Institute of Solid State and Materials Research)
Martin Friak (Max-Planck-Institut für Eisenforschung GmbH)
Suzana Fries (RWTH-Aachen)
Blazej Grabowski (Max-Planck-Institut für Eisenforschung GmbH)

Tilmann Hickel (Max-Planck-Institut für Eisenforschung GmbH)
Lars Ismer (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Adam Kiejna (University of Wroclaw)
Pavel Korzhavyi (Royal Institute of Technology)
Frank Lechermann (cole Polytechnique)
Petri Lethinen (Max-Planck-Institut für Eisenforschung GmbH)
Mark T. Lusk (Colorado School of Mines)
Liverios Lymperakis (Max-Planck-Institut für Eisenforschung GmbH)
Oliver Marquardt (Max-Planck-Institut für Eisenforschung GmbH)
Stefan Müller (Universitt Erlangen-Nürnberg)
Ashkan Naeini (SIEMENS AG, Corporate Technology)
Britta Nestler (Karlsruhe University of Applied Sciences)
Jörg Neugebauer (Max-Planck-Institut für Eisenforschung GmbH)
Duc Nguyen-Manh (Culham Science Centre)
Sergey Ostanin (University of Warwick)
Michal Petrov (Max-Planck-Institut für Eisenforschung GmbH)
Kriangyut Phiu-On (RWTH Aachen)
Matt Probert (University of York)
Andrei V. Ruban (Royal Institute of Technology)
Hans L. Skriver (Technical University of Denmark)
Mojmir Sob (Masaryk University, Brno)
Martin Stratmann (Max-Planck-Institut für Eisenforschung GmbH)
Julie D. Tucker (University of Wisconsin-Madison)
Ole Wieckhorst (Universitt Erlangen-Nürnberg)
Franois Willaime (CEA/Saclay)
Christopher Wolverton (Ford Research and Advanced Engineering)
Philippe Zeller (CEN Saclay)

3.2.2 Report on Workshop on *"The anomalous Hall effect: Recent advances via the geometric-phase approach"*

Organized by:
Raffaele Resta INFM-DEMOCRITOS National Simulation Center, Trieste, and Dept. of Theoretical Physics, University of Trieste Italy
Qian Niu University of Texas at Austin United States
Allan H. MacDonald University of Texas at Austin United States
held at:
CECAM 46 alle' e d'Italie 69007 Lyon France
from 2005-07-04 till 2005-07-06.

Supported by: Psi-k, CECAM.

Description

We plan to gather in Lyon about 20 senior condensed matter theorists, chosen among those who have contributed significant advances in understanding and computing : electric polarization, orbital magnetisation, anomalous Hall effect, quantum Hall effect, and Berry phases. Notably, we include scientitsts from a wider theoretical-physics community, A few junior participants will be invited later, depending on budget. The recent developments have occured at a very fast pace in the last two years. This workshop is intended as a very timely forum for discussing some of the unexplored links and consequences. The format and style of a CECAM workshop make the event ideal for discussing open and unsolved problems, work in progress, and other issues normally not reported in a formal talk at a larger (and less specific) conference.

Participant List

Taillefumier Mathieu (taillefu@mpi-halle.de), Max Planck institute Germany
Lacroix Claudine (lacroix@grenoble.cnrs.fr) CNRS France
Vitalii Dugaev (vdugaev@cfif.ist.utl.pt), Department of Physics and CFIF,
Instituto Superior Tecnico, Lisbon Portugal
Ivo Souza (isouza@berkeley.edu), University of California, Berkeley, United States
Guang-Yu Guo (gyguo@phys.ntu.edu.tw),National Taiwan University,
Department of Physics, Taipei 106 Taiwan, Republic of China
Andrea Dal Corso (dalcorso@sissa.it), SISSA Italy
Davide Ceresoli (ceresoli@sissa.it), SISSA Italy
David Vanderbilt (dhv@physics.rutgers.edu), Rutgers University United States
Yugui Yao (ygyao@aphy.iphy.ac.cn), Institute of Physics, Chinese Academy of Sciences China
Charles Kane (kane@physics.upenn.edu), University of Pennsylvania United States
Timo Thonhauser (timo.thonhauser@rutgers.edu), Rutgers, The State University of New Jersey

United States
Raffaele Resta (resta@democritos.it), INFM-DEMOCRITOS National Simulation Center, Trieste, and Dept. of Theoretical Physics, University of Trieste Italy
Patrick BRUNO (bruno@mpi-halle.de), Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle Germany
F. Duncan M. Haldane (haldane@princeton.edu), Princeton University United States
Allan H. MacDonald (macd@physics.utexas.edu), University of Texas at Austin United States
Tomas Jungwirth (jungw@fzu.cz), Institute of Physics ASCR, Prague and University of Nottingham Czech Republic
Qian Niu (niu@physics.utexas.edu), University of Texas at Austin United States
Francesco Mauri (Francesco.Mauri@lmcp.jussieu.fr), Universite Pierre et Marie Curie France
Ian Campbell (Ian.CAMPBELL@LCVN.univ-montp2.fr), Universite Montpellier II France
Carlo M. Canali (carlo.canali@hik.se), Kalmar University - Sweden Sweden
Jairo Sinova (sinova@physics.tamu.edu), Texas A&M University United States
Naoto Nagaosa (nagaosa@ap.t.u-tokyo.ac.jp), Department of Applied Physics, The University of Tokyo Japan

Presentation List

Anomalous Hall effect in a two-dimensional electron gas with spin-orbit interaction

Vitalii Dugaev
Department of Physics and CFIF, Instituto Superior Tecnico, Lisbon, Portugal

Abstract

We discuss the mechanism of anomalous Hall effect related to the contribution of electron states below the Fermi surface (induced by the Berry phase in momentum space). Our main calculations are made within a model of two-dimensional electron gas with spin-orbit interaction of the Rashba type, taking into account the scattering from impurities. We demonstrate that such an "intrinsic" mechanism can dominate but there is a competition with the impurity-scattering mechanism, related to the contribution of states in the vicinity of Fermi surface. We also show that the contribution to the Hall conductivity from electron states close to the Fermi surface has the intrinsic properties as well.

Chern numbers for ferromagnetic metal nanoparticles

Carlo M. Canali Kalmar University - Sweden, Sweden

Abstract

We argue that Ferromagnetic transition metal nanoparticles with fewer than approximately 100 atoms can be described by an effective Hamiltonian with a single giant spin degree of freedom. The total spin S of the effective Hamiltonian is specified by a Berry curvature Chern

number that characterizes the topologically non-trivial dependence of a nanoparticle's many-electron wavefunction on magnetization orientation. Interestingly, this simple procedure yields the correct Hund's-3rd-rule values for the ground state degeneracies for isolated (open-shell) atoms. The Berry curvatures and associated Chern numbers have a complex dependence on spin-orbit coupling in the nanoparticle and influence the semiclassical Landau-Liftshitz equations that describe magnetization orientation dynamics. Recent work to evaluate effective giant-spin Hamiltonians for realistic transition metal clusters by performing ab-initio calculations of the Berry curvatures will be discussed.

References:

C.M. Canali, A. Cehovin and A.H. MacDonald, Phys.Rev.Lett. 91, 046805 (2003).

Spin-orbit coupling, complex band structures and ballistic conductance with ultrasoft pseudopotentials

Andrea Dal Corso
SISSA, Italy

Abstract

The approach proposed by Choi and Ihm![1] for calculating the ballistic conductance of open quantum systems has been generalized to deal with magnetic transition metals described by ultrasoft pseudo-potentials.![2] I will present some results obtained recently with this method on the spin-resolved conductance of a model Ni nanocontact formed by a three atom monatomic wire placed between two tips made by seminfinite Ni slabs of (001) orientation.![3] Then, I will discuss how this approach can be generalized to treat systems described by spinor wavefunctions which allow to describe both non-collinear magnetic structures and systems with spin-orbit coupling.![4] As a first result, I will present the complex band structures of a Pt monatomic wire calculated accounting for spin-orbit effects.

References:

[1] H. J. Choi and J. Ihm, Phys. Rev. B 59, 2267 (1999).
[2] A. Smogunov, A. Dal Corso, and E. Tosatti, Phys. Rev. B 70, 045417 (2004).
[3] A. Smogunov, A. Dal Corso, and E. Tosatti, in preparation.
[4] A. Dal Corso and A. Mosca Conte, Phys. Rev. B 71, 115106 (2005).

Berry Phase Theory of Charge Effects in Insulators

David Vanderbilt
Rutgers University, United States

Abstract

I will first briefly summarize the Berry-phase theory of electric polarization, which is closely related to the theory of quantized adiabatic charge transport. I will mention some recent topics of interest, including the formulation of a theory of insulators in finite electric field in terms of a coupling of this field to the Berry-phase polarization, and the role of the Berry curvature and

metric and the relation of these to each other and to the degree of localization. Returning to the theory of polarization, I will discuss the need for an analogous theory of orbital magnetization, and I will discuss, in general terms, the similarities and differences that may be expected between these two theories.

Kohn localization and the quantum Hall effect

Raffaele Resta
INFM-DEMOCRITOS National Simulation Center, Trieste, and Dept. of Theoretical Physics, University of Trieste, Italy

Abstract

According to Kohn (1964) theory of the insulating state electron localization, defined in an appropriate sense, is the cause for the insulating behavior in any insulator. Since 1999 onwards, the theory of the insulating state has been reformulated in terms of a localization tensor which provides a measure of electron localization. This tensor is an intensive property, geometric in nature, which characterizes the ground wavefunction (not the individual states): it is finite in any insulator and divergent in any metal. In the special case of noninteracting electrons, the localization tensor of the insulating solid is related to the spherical second moment of the Wannier-function charge distribution. The localization tensor is a ground-state property, related via a fluctuation-dissipation theorem to the system conductivity. So far, the theory has only addressed systems with time-reversal symmetry, in which case the localization tensor is real. I show that in absence of such symmetry the localization tensor is naturally endowed with an imaginary part, proportional to transverse dc conductivity, and quantized in 2d systems. Therefore electron localization can be regarded as the common cause for both vanishing of the dc conductivity and quantization of the transverse one in QH fluids.

References:
W. Kohn, Theory of the insulating state, Phys. Rev. 133, A171 (1964);
R. Resta, Why are insulators insulating and metals conducting?, J. Phys.: Condens. Matter 14, R625 (2002);
R. Resta, Electron localization in the quantum Hall regime, cond-mat/0504054.

Orbital Magnetization in Extended Systems: Numerics and Results

Timo Thonhauser
Rutgers, The State University of New Jersey, United States

Abstract

We present tight-binding calculations of the orbital magnetization in chiral insulators. Our investigations focus on two-dimensional periodic systems with broken time-reversal symmetry and zero Chern number, and on finite samples cut from such systems. Time-reversal symmetry is broken by threading magnetic fluxes through parts of the unit cell in such a way that the net magnetic field remains zero. Results for the calculated magnetization as a function of the flux

show that, in the limit of large but finite systems, the orbital magnetization converges to its bulk value as computed in k-space using the formulation presented by Davide Ceresoli. Possible extensions to non-zero Chern numbers and metals will also be discussed.

References:

T. Thonhauser, Davide Ceresoli, David Vanderbilt, and R. Resta, submitted to PRL (cond-mat/0505518).

R. Resta, Davide Ceresoli, T. Thonhauser, and David Vanderbilt, ChemPhysChem, in press (2005).

Efficient ab initio calculation of the anomalous Hall conductivity by Wannier interpolation

Ivo Souza
University of California, Berkeley, United States

Abstract

The static intrinsic anomalous Hall conductivity is given by a Brillouin-zone integral of the Berry curvatures of the states below the Fermi surface. It is usually written as a Kubo-formula, which involves a sum over unoccupied states as well. Alternatively, it may be recast in a form where only occupied states appear explicitly. Finally, the non-quantized part can be expressed as a Fermi surface integral[1]. The only ab initio calculations so far[2,3] used the Kubo formula. I will discuss ideas for implementing the other two formulations. The first step is to map the ab initio electronic structure problem onto a tight-binding model, by constructing Wannier functions that accurately describe the ab initio band structure around the Fermi level[4]. The required quantities can then be evaluated very efficiently at arbitrary k points by Wannier interpolation, without having to perform aditional ab initio calculations. That is particularly advantageous for this problem, since an exceedingly fine sampling of certain regions of the Brillouin zone is needed in order to achieve convergence[3].

References:

[1] F. D. M. Haldane, Phys. Rev. Lett. 93, 206602 (2004).
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[3] Y. Yao et al., Phys. Rev. Lett. 92, 037204 (2004).
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Orbital Magnetization in Extended Systems: Theory

Davide Ceresoli
SISSA, Italy

Abstract

The magnetic dipole moment of any finite sample is well defined, while it becomes ill defined in the thermodynamic limit, due to the unboundedness of the position operator. The corresponding electrical problem, where surface charges and bulk polarization appear as entangled, has been solved about one decade ago by the modern theory of polarization, based on a Berry phase. We follow a similar path here, providing a bulk expression for orbital magnetization for any latticeperiodical, though time-reversal breaking, Hamiltonian. We therefore limit ourselves to cases where the macroscopic (i.e. cell-averaged) magnetic field vanishes. For crystalline insulators we express the bulk magnetization in terms of Wannier functions, and we then transform the expression into a Brillouin-zone integral involving the occupied Bloch orbitals. Interestingly, the final expression remains well-defined even for metals, but it is not yet clear whether it is correct in that case.

The Quantum Spin Hall Effect

Charles Kane
University of Pennsylvania, United States

Abstract

We show that the intrinsic spin orbit interaction in a single plane of graphene converts the ideal two dimensional semi metallic groundstate of graphene into a quantum spin Hall (QSH) state [1]. This novel electronic phase shares many similarities with the quantum Hall effect. It has a bulk excitation gap, but supports the transport of spin and charge in gapless "spin filtered" edge states on the sample boundary. We show that the QSH phase is associated with a Z_2 topological invariant, which distinguishes it from an ordinary insulator [2]. The Z_2 classification, which is defined for any time reversal invariant Hamiltonian with a bulk excitation gap, is analogous to the Chern number classification of the quantum Hall effect. We argue that the QSH phase is topologically stable with respect to weak interactions and disorder. The QSH phase exhibits a finite (though not quantized) dissipationless spin Hall conductance even in the presence of weak disorder, providing a new direction for realizing dissipationless spin transport.

References:

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[2] C.L. Kane and E.J. Mele, cond-mat/0506581

Spin Hall Effect and Spin Hall Spin Accumulation

Allan H. MacDonald
University of Texas at Austin, United States

Abstract

The controlled generation of localized spin-densities is a key enabler of semiconductor spintronics. Finite spin-densities in semiconductors have traditionally been generated by external magnetic fields, by circularly polarized light sources, or by spin injection from ferromagnetic metals.

Recently there has been considerable interest in an alternate strategy in which edge spin densities are generated electrically via the spin Hall effect, em i.e. (in a planar device) by the current of spins (j_H^z) oriented perpendicular to the plane that is generated by and flows perpendicular to an electric field. Practical interest in this effect is motivated by arguments that, at least in principle, it may enable low power consumption electronic devices. The spin Hall effect has traditionally been thought of as a consequence of skew-scattering, spin-dependent chirality in impurity scattering that ocurs in systems with spin-orbit coupling. Recently it has been recognized that the spin Hall effect also has an intrinsic contribution due to spin-orbit coupling in a perfect crystal. I will discuss the various contributions to the spin Hall conductivity and their relationship to the strongly analogous contributions the Hall conductivity of a ferromagnet. One broad classification of contributions is that the spin Hall conductivity is the sum of an interband coherence response contribution that is often dominated by an intrinsic part and a skew scattering contribution. In isotropic two-dimensional electron systems spin-orbit interactions can normally be modelled as momentum dependent Zeeman fields which always point in the plane. In these systems the skew scattering contribution is absent. For a two-dimensional hole gas with strong spin-orbit interactions the spin Hall conductivty is well approximated by its intrinsic contribution. The main observable consequence of the spin Hall effect is the spin accumulations near sample edges to which they give rise. Because spin is not conserved in systems with spin-orbit interactions, there is no unique definition of the spin current. The measure of merit of a particular spin-current definition is its utility for the evaluation of the edge spin accumulations associated with the spin Hall effect. There is not, as yet, a useful and general theory of these spin accumulations in systems with strong spin-orbit interactions. I will present and discuss numerical results which indicate that for a two-dimensional hole gas the edge spin-density is proportional to the spin Hall current and inversely proportional to the hole gas Fermi velocity, and that it is localized within a spin-precession length of the edge.

Disorder effects in Berry phase phenomena

Naoto Nagaosa
Department of Applied Physics, The University of Tokyo, Japan

Abstract

Disorder effects such as the impurity scattering play crucial roles in the transport phenomena and dielectric phenomena governed by the Berry phase curvature. Especially the debates on the intrinsic and extrinsic mechanism of anomalous Hall effect and spin Hall effect still continue with lots of confusions. I will talk on the recent advances on these problems. We found that the magnetic monopole and the associated non-perturbative aspect is essential for the intrinsic mechanism. I will also discuss the role of Anderson localization in anomalous Hall effect and charge pumping.

Pseudopotential Hamiltonian in Magnetic field: the orbital magnetism within a pseudopotential framework

Francesco Mauri
Universite Pierre et Marie Curie, France

Anomalous Hall Effect in Ferromagnets

Patrick BRUNO
Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

Berry Phase Theory of the Anomalous Hall Effect

F. Duncan, M. Haldane
Princeton University, United States

Abstract

The Karplus-Luttinger formula for the intrisic AHE has been recognized as an integral over the "Berry Curvature" of all occupied Bloch states. This formula resembles the Landau diamagnetism formula, and appears not to be a Fermi surface formula, in violation of the fundamental principle that all transport processes occur at the Fermi level. Recently I have shown that it is in fact the sum of a quantized part associated with topologically-non-trivial occupied bands, and non-quantized part determined entirely at the (bulk) Fermi surface. There is a simple geometrical formula for the Fermi surface part that is valid in interacting Fermi liquids (like the Luttinger Fermi surface volume theorem, to which it is related); the quantized part is also a Fermi level effect associated with chiral edge states at the Fermi level, which are necessaily present if there are fully-occupied bands with non-trivial topology. These results prompt a new look at ingredients of Fermi liquid theory that were not recognized when that theory was developed. A subtlety about the "Berry curvature" of Bloch states will also be discussed: it encodes the embedding of Hilbert space in real space in addition to properties of the Bloch wavefunctions.

References:

F. D. M. Haldane, Phys. Rev Lett. 93, 206602 (2004)

Berry phase correction to electron density of states in solids

Qian Niu
University of Texas at Austin, United States

Abstract

Liouville's theorem on the conservation of phase space volume is violated by Berry phase in the semiclassical dynamics of Bloch electrons. This leads to a modification of the phase space density of states, whose significance is discussed in a number of examples: field modification of the Fermi-sea volume, connection to the anomalous Hall effect, and a general formula for orbital magnetization. The effective quantum mechanics of Bloch electrons is also sketched, where the modified density of states plays an essential role.

On a Proper Definition of Spin Current

Qian Niu
University of Texas at Austin, United States

Abstract

The conventional definition of spin current is incomplete and unphysical in describing spin transport in systems with spin-orbit coupling. A proper and measurable spin current is established in this study, which fits well into the standard framework of near-equilibrium transport theory and has the desirable property to vanish in insulators with localized orbitals. Our theory predicts opposite signs of spin Hall coefficients for a few semiconductor models, urging critical tests of the concept by experiments and numerics.

Ab initio calculation of spin Hall effect in semiconductors and anomalous Hall effect in ferromagnetic insulators

Guang-Yu Guo
National Taiwan University, Department of Physics, Taipei 106, Taiwan, Republic of China

Abstract

Spin current generation is an important issue in the emerging spintronics technology. Recent proposals of the intrinsic spin Hall effect by Murakami et al [1] and Sinova et al [2], are therefore fascinating. This spin Hall effect would enable spin current generation in semiconductors without magnetic field or magnetic materials, and promise a tremendous potential of combining spintronics with the well-developed semiconductor technology. However, the recent proposals of the intrinsic spin Hall effect have been subject to careful scrutinies. In particular, Wang and Zhang [3] argued that spin symmetry consideration would rule out the possibility of such a spin current in the semiconductors described by the Luttinger Hamiltonian which was used in [1]. On the other hand, Zhang and Yang [4] point out that the intrinsic spin Hall effect predicted in [2], in a two-dimensional electron gas in semicoductors, would be exactly cancelled by the intrinsic orbital-angular-momentum Hall (orbital) effect. Therefore, fundamental questions such as the existence of the intrinsice spin Hall effect in semiconductors structures and that whether it would be cancelled out by the orbital Hall effect, remain unsolved despite enormous recent efforts. In this talk, we report our ab initio relativistic band theoretical calculations on the intrinsic spin Hall effect in the archetypical semiconductors Si, Ge, GaAs and AlAs [5]. Our results cover a large range of hole concentration which is beyond the validity regime of the Luttinger model. We find that intrinsic spin Hall conductivity in hole-doped semiconductors Ge, GaAl and AlAs is large, showing the possibility of spin Hall effect beyond the Luttinger Hamiltonian. The calculated orbital Hall conductivity is one order of magnitude smaller, indicating no cancellation between the spin and orbital Hall effects in bulk semiconductors. Furthermore, it is found that the spin Hall effect can be strongly manipulated by strains, and that the ac spin Hall conductivity in the semiconductors is large in pure and as well as doped semiconductors.

References

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Spin Hall Effect

Tomas Jungwirth
Institute of Physics ASCR, Prague and University of Nottingham, Czech Republic

Spin Hall Effect

Jairo Sinova
Texas A&M University, United States

The anomalous Hall effect in re-entrant AuF alloys and the real space Berry phase

Ian Campbell
Universite Montpellier II, France

Abstract

The Hall effect has been studied in a series of AuFe samples in the re-entrant concentration range, as well as in the spin glass range. The data demonstrate that the degree of canting of the local spins strongly modifies the anomalous Hall effect, in agreement with model predictions associating canting, chirality and the "real space Berry phase". The canonical parametrization of the Hall signal for magnetic conductors becomes inappropriate when local spins are canted.

Program

Day 1: July 04 2005

Session	:	1 **Anomalous Hall effect**	
09:00 to 09:30	:	Welcome	
09:30 to 10:30	:	Anomalous Hall Effect in Ferromagnets	Patrick BRUNO
10:30 to 11:00	:	Coffee Break	
11:00 to 12:00	:	Berry Phase Theory of the Anomalous Hall Effect	F. Duncan M. Haldane

Session	:	**2 Orbital magnetization**	
14:00 to 15:00	:	Berry Phase Theory of Charge Effects in Insulators	David Vanderbilt
15:00 to 15:15	:	Orbital Magnetization in Extended Systems: Theory	Davide Ceresoli
15:15 to 15:30	:	Orbital Magnetization in Extended Systems: Numerics and Results	Timo Thonhauser
15:30 to 16:00	:	Coffee Break	
16:30 to 16:50	:	Pseudopotential Hamiltonian in Magnetic field: the orbital magnetism within a pseudopotential framework	Francesco Mauri
16:50 to 18:00	:	Discussion	
16:00 to 16:30	:	Berry phase correction to electron density of states in solids	Qian Niu

Day 2: July 05 2005

Session	:	**3 Spin Hall effect**	
09:00 to 10:00	:	Spin Hall Effect and Spin Hall Spin Accumulation	Allan H. MacDonald
10:00 to 10:30	:	The Quantum Spin Hall Effect	Charles Kane
10:30 to 11:00	:	Coffee Break	
11:00 to 11:30	:	Ab initio calculation of spin Hall effect in semiconductors and anomalous Hall effect in ferromagnetic insulators	Guang-Yu Guo
11:30 to 11:45	:	Spin Hall Effect	Tomas Jungwirth
11:45 to 12:00	:	Spin Hall Effect	Jairo Sinova

Session	:	**4 Spin currents; localization**	
14:00 to 14:30	:	On A Proper Definition of Spin Current	Qian Niu
14:30 to 15:00	:	Discussion	
15:00 to 15:30	:	Coffee Break	
15:30 to 16:00	:	Kohn localization and the quantum Hall effect	Raffaele Resta
16:00 to 16:30	:	Efficient ab initio calculation of the anomalous Hall conductivity by Wannier interpolation	Ivo Souza
16:30 to 17:00	:	Chern numbers for ferromagnetic metal nanoparticles	Carlo M. Canali

Day 3: July 06 2005

Session	:	**5 Disorder; spin-orbit**	
09:00 to 10:00	:	Disorder effects in Berry phase phenomena	Naoto Nagaosa
10:00 to 10:30	:	The anomalous Hall effect in re-entrant AuF alloys and the real space Berry phase	Ian Campbell
10:30 to 11:00	:	Coffee Break	
11:00 to 11:30	:	Spin-orbit coupling, complex band structures and ballistic conductance with ultrasoft pseudopotentials	Andrea Dal Corso
11:30 to 12:00	:	Anomalous Hall effect in a two-dimensional electron gas with spin-orbit interaction	Vitalii Dugaev

Organizer's report

Conclusions

There have been sweeping advances since 2002 in understanding and computing the anomalous Hall effect (AHE) from first principles. The Hall resistivity of ferromagnets has an ordinary contribution (proportional to the external magnetic field strength), and an anomalous contribution (often assumed proportional to the sample magnetization). The phenomenon of AHE was discovered by E.R. Hall in 1881, shortly after his discovery of the normal effect. Nonetheless its interpretation has been controversial until recently. It is by now clear that the AHE is dominated by band-structure effects and can be computed as a suitable Berry phase. Other closely related, and equally controversial issues, concern the spin Hall effect, and orbital magnetization in extended systems. All of these issues have possible relevant implications for spintronics applications. The above topics have been thoroughly and lively discussed in the workshop. Besides the "formal" presentations, an important part of the meeting has been in the long discussions, augmented with a few informal short presentations. We have gathered in Lyon 21 condensed matter theorists (plus a senior experimentalist), chosen among those who have in the past contributed significant advances in understanding and computing: electric polarization, orbital magnetization, anomalous Hall effect, quantum Hall effect, and Berry phases. Notably, we included scientists from the computational electronic-structure community, as well as scientists from a wider theoretical-physics community. It is remarkable that, while the preliminary participants' list was built on the basis of a generic cultural interest, some people in this list started working more specifically on the workshop topics only AFTER the workshop was proposed and approved. Given the nature of the event, most participants were senior ones, where some junior collaborators of the senior participants attended as well. Two young US participants profited of the NSF support under the CECAM-NSF agreement. Some participants, including the most seniors of them, sent a feedback of real enthusiasm. It is remarkable that-despite the partial support available under the CECAM rules-almost one half of the participants travelled from overseas (USA, Japan, Taiwan) expressly for this very short event. The success of the workshop owes to two main features. (1) Timeliness, demonstrated by the fact that a large number of important papers (e.g. PRLs), and preprints posted on the web, have appeared AFTER the workshop was proposed and approved. (2) By means of participants' selection, care was taken to foster the interaction between physicists belonging to different communities: quantum-Hall (mostly analytical approach) and electronic structure (mostly computational approach).

3.2.3 Report on Workshop on "Data representation and code interoperability for computational materials physics and chemistry"

CECAM, Lyon (France)

April 19-21, 2006

Sponsored by CECAM, Psik,

and the ESF-EUROCORES programme "EuroMinScI"

Organizers:

Alberto Garcia (Universidad del Pais Vasco, Bilbao, Spain)

Phil Couch (CCLRC-Daresbury Laboratory, UK)

Thomas Schulthess (Oak Ridge National Laboratory, USA)

The computational approach to the study of matter has been hugely successful, but this success has brought some practical problems. On the one hand, the inmense amounts of data generated need to be analyzed and/or archived and catalogued for later retrieval or distribution. On the other, it is sometimes desirable to study the same system with various codes which implement different features or levels of approximation (e.g. a tight-binding calculation followed by an ab-initio one). Currently, the input/output formats of the vast majority of codes are completely different, even if they refer to magnitudes (i.e., atomic coordinates, charge densities) which are perfectly well characterized from the physical point of view.

This workshop was devoted to the use of data representation tools (basically XML and related technologies) in atomistic simulations, with an emphasis on the needs of the electronic structure community in regard to interoperability of codes and ease of post-processing of results.

This event was made possible thanks to partial support from:

- **CECAM**
- **The Psik network**
- **The European Science Foundation** (ESF) under the EUROCORES Programme **EuroMinScI**, through contract No. ERAS-CT-2003-980409 of the European Commission, DG Research, FP6.

Workshop Conclusions

1. The workshop highlighted several key motivations for the development of a data management framework and these are summarised below.

- *Interoperability*
  Increasingly, addressing many scientific problems requires the use of more than one application used in close co-operation. For example, often, any attempt to bridge length and time scales requires a hybrid of classical and quantum mechanical methods or the application of various levels of theory. Such approaches could be implemented as a workflow, with information being exchanged between various simulation codes. The control of such complexity mandates a coherent approach to the management of data.
- *Visualisation and analysis*
  Considerable effort is invested in the development of tools that can be used to analyse and visualise simulation results. Unfortunately, these tools are often restricted to use with specific applications.
- *Data longevity*
  Currently, it is often quicker to duplicate effort regenerating simulation results than to locate and retrieve existing results from a repository; data longevity requires serious consideration.
- *Data volume*
  Data are generated at ever increasing rates and methods for dealing with large volumes of data from both experiment and simulation are required.
- *Efficient use of future computer resources*
  The present computing paradigms don't scale well. The development of data organisation strategies will be key for efficient use of the next generation of machines.

2. A number of groups have started their own efforts toward structured data handling. In the process, several useful tools have appeared. This workshop has served in part as a useful showcase of those efforts and developments. Most work has been done with XML, although there have been important advances in the handling of large binary data sets in portable formats (netCDF, HDF5). Among the XML efforts, the chemical markup language (CML) figures prominently in several projects, while other groups have designed their own data markups.

3. A global standard for data formats in chemistry and materials science is not realistic or practical at present. On the other hand, convergence in narrower domains, and the initial adoption of data representation concepts and tools by most codes might be within reach in the short to medium term.

4. An ontology-mediated approach (that involves the specification of relevant concepts within a given domain) could provide an initial alternative to defining a common global representation for data. Such an approach will allow interoperability between communities that work with different data models and that use different technologies (i.e. XML, relational databases, netCDF/ HDF5).

5. Once well-defined ontologies and data structures with manageable scope are created, a mixed process of federation, nucleation around proven ideas, and pruning of redundant material could potentially result in a successful global schema.

Workshop Recommendations

1. Encourage code developers to look into existing tools for data representation, even if only at the single-code level. The creation of some form of structured data is already a significant step for interoperability, as automatic transformation is in principle possible.
2. Form special-interest groups associated to specific domains for which potential global schema for data structures could be drafted. During the workshop the following domains and people involved were identified:
    - (Molecular) orbitals and basis sets: Knowles, Baldridge, Rossi, Sherwood, Fawzi, Kim, Garcia.
    - Monte-Carlo data: Troyer, Kim,Schulthess.
    - Large binary data (in quantum chemistry and electronic structure): Rossi, Gygi, Fawzi, Garcia.
    - LMTO data sets: Schulthess, Temmerman.
3. Create an infrastructure to serve as follow-up to the workshop and as the basis for future collaboration. The workshop website at www.cecam.fr was used initially to hold the actual workshop material, but immediately afterwards a new Twiki site (www.datarepresentation.org, maintained by P. Sherwood and P. Couch) was created as a more focused and longer-lasting resource to hold links and discuss best practices.
4. Assign initial follow-up tasks
    - Develop a tutorial on dictionaries and schemas: Murray-Rust.
    - Organize an access-grid follow-up meeting a few months after the workshop: Sherwood.
    - Create a table in which input data fields and their use in various condensed-matter electronic structure methods are analyzed: Schulthess, Gonze, Gygi.
5. In the longer term, the community should look into ways to maintain the momentum to develop better data representation frameworks and tools. It seems that there is a good enough case to justify one or several funding applications. There should be a follow-up workshop in about 2 years.

Program

Day 1: April 19 2006

Session : 1 Introduction and Showcase-1
09:00 to 09:10 : Welcome
Alberto Garcia

09:10 to 09:40 : Presentation
Information Exchange in Computational Chemistry and Materials Physics - An Overview
Phil Couch

09:40 to 10:10 : Presentation
Overview of CML
Peter Murray-Rust

10:10 to 10:40 : Presentation
MaterialsGrid and CML
Daniel Wilson

10:40 to 11:10 : Presentation
XML I/O Subsystem for Computational Nanoscience
Thomas Schulthess

11:10 to 11:30 : Coffee Break

Session : 2 Showcase-2
11:30 to 12:00 : Presentation
Grid Enabled Molecular Science Through Online Networked Environments
Kim Baldridge

12:00 to 12:30 : Presentation
Automatically extracting metadata from CML for combinatorial simulations on the grid
Richard Bruin

12:30 to 13:00 : Presentation
On the structuring of the computational chemistry Virtual Organization COMPCHEM
Osvaldo Gervasi

13:00 to 14:30 : Lunch Break

Session : 3 Ongoing efforts in data formats
14:30 to 15:00 : Presentation
Specification of file formats for NANOQUANTA
Xavier Gonze

15:00 to 15:30 : Presentation
A proposal for a unified norm-conserving pseudopotential format
Javier Junquera

15:30 to 16:00 : Presentation

Data file exchange in Quantum-ESPRESSO
Paolo Giannozzi

16:00 to 16:30 : Presentation
Data representation for biomolecular systems: technical and political challenges
Konrad Hinsen

16:30 to 17:00 : Coffee Break

Session : 4 Demonstration-1
17:00 to 17:30 : Presentation
Demonstration of XML tools: xmlf90
Jon Wakelin

17:30 to 18:00 : Presentation
XSLT transforms
Toby White

Day 2: April 20 2006

Session : 1 Electronic Structure Codes
09:00 to 09:30 : Presentation
XML Schema Design for First-Principles Molecular Dynamics
Francois Gygi

09:30 to 10:00 : Presentation
Object representations for quantum simulations
Jeongnim Kim

10:00 to 10:30 : Presentation
The ALPS project
Matthias Troyer

10:30 to 11:00 : Presentation
Unified XML I/O approach in DFT and model codes for real materials: from crystal structure to magnetic susceptibility
Anton Kozhevnikov

11:00 to 11:30 : Coffee Break

Session : 2 Quantum Chemistry Codes
11:30 to 12:00 : Presentation

Data representation in the Molpro quantum chemistry package
Peter Knowles

12:00 to 12:30 : Presentation
A common format for Quantum Chemistry
Elda Rossi

12:30 to 13:00 : Presentation
Building an Infrastructure for Quantum Chemistry: Data Sharing and Graphical User Interfaces
Paul Sherwood

13:00 to 13:30 : Lunch Break

Session : 3 Discussion session 1
14:30 to 15:00 : Presentation
Material leading to discussion: Data markup hierarchies and interoperation
Peter Murray-Rust

15:00 to 16:30 : Discussion

16:30 to 17:00 : Coffee Break

Session : 4 Demonstration-2
17:00 to 18:00 : Presentation
An Introduction to the Use of XMLDIR and QuickSchema
Michael Summers

Session : 5 Social dinner
Day 3: April 21 2006

Session : 1 Other Tools
09:00 to 09:30 : Presentation
XML and the Vienna Ab-initio Simulation Package (VASP)
Orest Dubay

09:30 to 10:00 : Presentation
Information Exchange in Computational Chemistry and Materials Physics - AgentX
Phil Couch

10:00 to 10:30 : Presentation
Evolutionary Construction of Higher-level Constraints over an XML Language; Formalizing Informal Semantics

Toby White

10:30 to 11:00 : Presentation
CCPN - automatic code generation from UML data models
Rasmus Fogh

11:00 to 11:30 : Coffee Break

Session : 2 Other issues
11:30 to 12:00 : Presentation
Handling of large datasets in Quantum Chemistry
Antonio Monari

12:00 to 12:30 : Presentation
Input handling in CP2K
Fawzi Roberto Mohamed

12:30 to 13:00 : Discussion

13:00 to 14:30 : Lunch Break

Session : 3 Discussion-2
14:30 to 16:30 : Discussion

16:30 to 17:00 : Coffee Break

Session : 4 Concluding remarks and hands-on session
17:00 to 18:00 : Discussion

Presentation List

Information Exchange in Computational Chemistry and Materials Physics - An Overview

Phil Couch

CCLRC-Daresbury Laboratory, United Kingdom

Abstract

A lack of information management in computational chemistry and materials physics is hindering progress in a number of important areas. Increasingly, addressing scientific problems requires a mixture of simulations codes used in close cooperation. As a result, considerable effort has been applied to the development of general tools that can be used to specify and execute complex computational workflows. Unfortunately, it is difficult to realise the full potential of these tools due to a lack of data standards. It is simply not possible to exchange information seamlessly and in an automated fashion between workflow components; format convertors and wrappers must be developed prior to execution. Such information exchange between simulation codes and tools that can be used to visualise and analyse data would also be an important development; common tools could be created to work with a range of simulation codes. The XML standards provide a good starting point for the development of our own data standards; they are mature and generally well adopted. This presentation details the requirements of a common XML data model and looks at how different data model designs meet these. Several common approaches for manipulating XML data from simulation codes are emerging; many building upon others. A summary of the different approaches with their corresponding strengths and weaknesses will be presented.

Overview of CML

Peter Murray-Rust
Unilever Ctr for Mol. Informatics, U. of Cambridge, United Kingdom

Abstract

- CML is now a robust technology which can support a large variety of concepts in computational chemistry and physics.

- It is designed as a core architecture with controlled XML syntax but high extensible through the use of dictionaries.

- These dictionaries are closely linked to individual codes which allows developers to work independently. Many dictionaries can be used simultaneously and this allows a model where dictionaries can later be merged and refactored to represent consensus in the community.

- A core dictionary for scientific units has been developed and this allows developers to translate units between different codes.

- A recent development is that CML documents (and therefore programs) can be validated through the JUMBO software. This has been done for output from CASTEP, SIESTA and DL_POLY.

- Developments in XML-CML include: (a) archiving of computational results in institutional repositories (b) engagement with STM publishers about direct publication of results (c) high-throughput analysis of computational chemistry results. (d) response to community demands - e.g. balancing markup vs speed, descriptions of extended objects, etc.

MaterialsGrid and CML

Daniel Wilson
Univ. of Frankfurt, Germany

Coauthors: Andrew Walkingshaw, Bjorn Winkler, Martin Dove, Peter Murray-Rust

Abstract

MaterialsGrid is a new project involving the Universities of Frankfurt and Cambridge, Accelrys, IBM, and the Central Laboratory of the Research Councils in the UK (CCLRC), which is funded by the UK government, and aims to create a pilot database of materials properties (such as elastic stiffness, dielectric constants, optical properties, heat capacity, electronic band gap) based on quantum mechanical simulations.

Central to the project is the idea that the database should be dynamic. Consequently, the front-end, data and compute infrastructures will be linked so that calculations will be triggered automatically if gaps are found in the data. Rather than use proprietary file formats, we use CML for all internal communication, as this allows us to use any CML-aware code as the computational chemistry 'engine'.

In this contribution, I will discuss the MaterialsGrid project, paying particular attention to the role of CML. I will also discuss our initial ontological analysis, and the implementation details of our CML-aware version of CASTEP. Furthermore, work within our group on the development of CML dictionaries will be presented.

XML I/O Subsystem for Computational Nanoscience

Thomas Schulthess

Oak Ridge National Laboratory, United States

Coauthors: M. Summers, A. Kozhevnikov, F. Rose, J. Velev, A. Janoti

Abstract

Nanoscience is typical for science of the 21st century in that it is very interdisciplinary, combining traditional domains such as physics, chemistry, materials science, and biology. Computational nanoscience can build on highly sophisticated techniques that have been developed in the respective domains. The interdisciplinary nature of the field, however, requires scientists to apply very different computational methods and codes that have been developed independently over decades. Furthermore, computational nanoscience relies increasingly on leading high performance computing platforms that are becoming increasingly more complex, requiring specialization of software systems. Finally, software systems have to be highly configurable, since nanoscience is a rapidly developing field. In a nutshell, the following characteristics are typical for computational nanoscience:

- 1. Interoperability of codes that have been developed independently.
- 2. Use of customized highly optimized codes for particular computing architectures.
- 3. Flexibility and extensibility of the software system
- 4. Ability to incorporate legacy codes

¿From the point of view of data representations, this requires that input and output data formats are as unique as possible across different codes, or, at a minimum, defined in a way that they can be easily translated. The use of XML to express data and metadata is therefore a very natural and appropriate choice for many situations. However, in order to make XML based technology work in real application, we have to address several challenges:

- 1. Parsing and validation must be supported for various flavors of Fortran, in addition to C and C++, without the need for heroic rewriting of codes
- 2. The XML technology must be usable on high performance computing platforms.
- 3. Consensus on XML Schemas must be developed by code developers as well as users.

In this talk I will give an overview of the XML I/O subsystem, the tools, and the Schema development environment that we are implementing at ORNL. In the morning of Day 2 of the workshop, Anton Kozhevnikov will discuss how the XML I/O subsystem has been incorporated into the Stuttgart LMTO code and how this has enabled him to combined electronic structure calculations with model Hamiltonian simulations that use the ALPS toolkit (see also talk by Matthias Troyer in the same session). In a later talk on day 2, Michael Summers will give detailed introduction and demonstration of the XML I/O subsystem.

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Grid Enabled Molecular Science Through Online Networked Environments

Kim Baldridge
Uni Zurich, Organic Chemistry Institute, Switzerland
Coauthors: Karan Bhatia, Steve Mock, Jerry Greenberg

Abstract

GEMSTONE (Grid Enabled Molecular Science Through Online Networked Environments), is a cross-platform desktop application that provides users access to remote scientific web services, with emphasis in this work for computational chemistry and biochemistry applications. Gemstone is built upon the Mozilla foundation codebase and available as a Firefox extension, with automatic update of new releases. The new infrastructure is capable of providing a versatile desktop user interface to strongly typed web services for applications running in a distributed cluster computing environment. The user interface enables a user to save and reuse application parameters, with drag and drop capability on multiple platforms. The interface supports server-side dynamic user interface configuration update. First phase Gemstone implimentation provides support for applications such as Adaptive Poisson-Boltzmann Solver (APBS), Babel, GAMESS (General Atomic and Molecular Electronic Structure System), a visualization component, GARNET, as well as several small interface tools that have been rewrapped to be web services. Additional applications are in the works, being easily added using the Gemstone application support framework, an integrated framework for accessing grid resources that supports scientific exploration, workflow capture and replay, and a dynamic services oriented architecture.

An outcome of this work has been the generation of an automatic web service wrapper, OPAL, which enables one to wrap legacy applications as Web services for deployment of applications as Web services in a matter of hours. This talk will show these efforts.

Automatically extracting metadata from CML for combinatorial simulations on the grid

Richard Bruin

Dept. of Earth Sciences, Univ. of Cambridge, United Kingdom

Abstract

As grid computing becomes more mainstream and scientists are able to submit larger number of calculations to be performed concurrently the difficulties faced by the scientist change dramatically. The difficulties move from "where can I find a machine to run my job?" to being " can run so many jobs now, how do I handle all of the data created?" I will describe how the eMinerals project uses CML program output for automatic collection of metadata. Our simulation codes (which include SIESTA and DL_POLY) generate three main types of CML output: metadata associated with the running of the program (eg program name, version number etc), parameters associated with the control of the simulation (such as temperature or pressure, function cut offs etc), and key properties (such as average volume and final energy). We typically run these programs within a grid computing environment. I will describe the job submission procedures we have developed, which now include tools based on the Agent-X and RCommand libraries developed by CCLRC, and give some case studies.

On the structuring of the computational chemistry Virtual Organization COMPCHEM

Osvaldo Gervasi

Coauthors: Antonio Lagana, Antonio Riganelli

University of Perugia, Dept. of Maths and Comp Sci, Italy

Abstract

The first moves to structure the COMPCHEM (Computational Chemistry and Molecular sciences) virtual organization (VO) of the related sientific community are discussed. The efforts have been focused on the assemblage of a grid enabled molecular simulator (GEMS) by gathering together the human, hardware and software resources of several research laboratories. To this end the necessary suites of codes have been structured in a way to operate in a distributed coordinated way on an extended grid of computers. A particularly critical point has been found to be the sustainability of such an effort.

Specification of file formats for NANOQUANTA

Xavier Gonze
Universite Catholique de Louvain, Belgium
Coauthors: C.-O. Almbladh, A. Cucca, M. Marques, C. Freysoldt, V. Olevano, Y. Pouillon, M. Verstraete

Abstract

In order to allow softwares to interact and exchange data, file format specifications are mandatory. Widely agreed file format specifications are still lacking in the field of first-principles calculations of material properties.

One of the (numerous) objectives of the European Network of Excellence "NANOQUANTA" is precisely to specify file formats, for the contents that are relevant to the scientific activity of its constituting nodes. After one year and a half of existence of NANOQUANTA, a large body of work has been done along these lines. It includes an inventary of the different contents, discussions of existing formats when relevant, as well as detailed (new) NetCDF specifications, for selected contents (density/wavefunctions). Pseudopotentials and geometry descriptions have also been examined. A document has been written, that gives specifications for the NANOQUANTA groups. It is hoped that the new specifications will be implemented in many different softwares, or (at least) will be the basis of even better file format specifications

A proposal for a unified norm-conserving pseudopotential format

Javier Junquera
Univ. Cantabria, Spain, Spain
Coauthors: Alberto Garcia and Matthieu Verstraete

Abstract

Pseudopotentials are widely used in electronic structure calculations and first-principles molecular dynamics simulations. At the present time, however, each computer code uses its own format for the input of pseudopotential information, which hinders interoperability and makes it difficult to compare the results obtained with different programs. Here we present a proposal for a unified file format for norm-conserving pseudopotentials. The new format is based on XML, and thus platform independent and easily processed by a wide variety of off-the-shelf tools, including a new Fortran XML parser (see http://lcdx00.wm.lc.ehu.es/ag/xml). This means that first-principles codes using pseudopotentials can easily map the information in the XML file to their internal data structures. While the current proposal is limited to norm-conserving pseudopotentials, it offers a proof-of-concept for the general approach. Further discussion and development is ongoing under the auspices of the FSAtom project (http://dirac.cnrs-orleans.fr/fsatom_wiki/PseudoPotentials).

Data file exchange in Quantum-ESPRESSO

Paolo Giannozzi
Scuola Normale Superiore di Pisa , Italy

Abstract

The need to extract and process information (wavefunctions, charge density etc) from data files produced by electronic structure codes is strongly felt in the scientific community. In this talk I will describe the state of the art and the perspectives of data file exchange in the Quantum-ESPRESSO distribution. The goal is to make access to data files produced by QE codes as easy as possible. The ideal data file format should satisfy several different and sometimes conflicting requirements: - fast to read and write - easy to read, parse and write without special libraries - easy to understand, self-documented - portable across different computer architectures - portable across different software packages The solution we have devised uses a data directory, instead of a single file, thus exploiting the capabilities of the file system for data organization. Binary I/O is used for large records (wavefunctions, charge density) while smaller records (for instance, the structure and symmetry of the system, the pseudopotentials) are written to a XML file (formatted). A small specialized library (iotk, input/output toolkit written by G. Bussi) is used to write and read the XML files and records.

Data representation for biomolecular systems: technical and political challenges

Konrad Hinsen
Laboratoire Lé on Brillouin (CEA-CNRS), France

Abstract

Biomolecular simulations are characterised by complex data structures, large data sets, and the need to interface with equally complex experimental data. The existence of few big simulation packages with relatively closed user communities has so far discouraged any efforts towards interoperatibility, except for the representation of molecular structures, which are the main interface to experiment. I will give an overview of the data for which a standardized representation would be desirable, either for interoperability or for archiving, and discuss the criteria that should be taken into account when defining file formats. I will also report on recent attempts at reaching a concensus about interoperability and why they have failed so far.

References

[1] Hinsen, K. *The Molecular Modeling Toolkit: A New Approach to Molecular Simulations*, J. Comp. Chem. **21** 79-85 (2000)

Demonstration of XML tools: xmlf90

Jon Wakelin
University of Bristol, UK, United Kingdom
Coauthors: Toby White, Alberto Garcia

Abstract

XML is a common solution to problems of transferable data exchange, and code interoperability. However, current codes must be moved into the XML world. One option is pre/post-processing of existing formats, but a more direct method is integrating XML into the code itself. Many such scientific codes are written in Fortran - to this end xmlf90 is a modern Fortran library which facilitates XML input (parsing) and output. Parsing can be done within the SAX and DOM paradigms. In addition, xmlf90 has a specialized module for CML code to facilitate output of well-structured, semantically full CML documents, in a fashion non-intrusive and comprehensible to the scientific programmer unversed in XML technologies.

XSLT transforms

Toby White
Dept. of Earth Sciences, Univ. of Cambridge, United Kingdom
Coauthor: Jon Wakelin

Abstract

XSLT transforms allow the manipulation of XML data in a platform-independent, programming-language-agnostic manner. Here I illustrate two applications of XSLT transforms of real and practical use. Firstly, generation of useful, human readable, visual output from a non-application-specific CML file. A mixed-namespace XHTML/CML/SVG output file is shown, visualizable in any standards-conformant WWW browser, which includes 2D SVG graphs of quantities of interest, and 3D embedded visualizations (via Jmol) of molecular structures. (i) Of particular interest is the Jmol integration, which entailed additions to the Jmol codebase to allow Jmol to directly traverse the namespace XML document in which it is embedded and extract relevant CML data. (ii) Also of interest is the graph-drawing XSLT which, in a fully general fashion, will extract and draw 2D graphs of arbitrary scale.

XML Schema Design for First-Principles Molecular Dynamics

Francois Gygi
University of California, Davis, United States

Abstract

First-Principles Molecular Dynamics (FPMD) simulations are rapidly gaining importance in many areas of computational materials science, physics and chemistry. This is accompanied by a growing need to facilitate data exchange between FPMD simulation codes and post-processing tools or other simulation codes such as quantum Monte-Carlo codes. XML is emerging as the best candidate markup language for exchange of FPMD data. The use of XML must be supplemented with a definition of elements and attributes used to markup FPMD data. This can be done using the older Document Type Definition (DTD) syntax, or with the more powerful XML Schema language. We present an XML Schema definition of FPMD simulation data. This definition has been used successfully by the Qbox plane-wave, pseudopotential FPMD code for

over two years. We discuss general rules that were followed in the design of the FPMD XML Schema specification. Semantic conflicts with other XML definitions are avoided through the use of XML namespaces. The use of a well defined XML syntax for FPMD simulation leads to improved reliability of simulation data since XML FPMD documents can be validated against their corresponding XML Schema definition and processed using extended stylesheet language transformations (XSLT). These properties will be illustrated with examples taken from the use of the Qbox code.

Object representations for quantum simulations

Jeongnim Kim

NCSA, United States

Abstract

I present recent developments of object representations for quantum simulations in the context of Quantum Monte Carlo (QMC) simulations and tools to interface multiple applications. We have developed qmcPACK (Quantum Monte Carlo Package) in an object-oriented framework. qmcPACK exploits the natural mapping between the computational objects and the data representation in xml. I discuss QMC schema and QMC applications, focusing on i) the data representation to facilitate data exchange with other applications and ii) the execution model to perform QMC simulations with many run-time parameters.

The ALPS project

Matthias Troyer

Theoretische Physik, ETH Zürich , Switzerland

Abstract

The ALPS project (Algorithms and Libraries for Physics Simulations) is an open source effort aiming at providing high-end simulation codes for strongly correlated quantum mechanical systems as well as C++ libraries for simplifying the development of such code. ALPS strives to increase software reuse in the physics community.

Unified XML I/O approach in DFT and model codes for real materials: from crystal structure to magnetic susceptibility

Anton Kozhevnikov

Russian Acad. Sciences, Russia, Russian Federation

Abstract

We report progress in implementing XML I/O in the TB-LMTO-ASA band structure code. Parsing and validation of xml source as well as modification and saving of DOM tree were done with the Xerces/Xalan libraries. The XML I/O paradigm was then used in calculations of Heisenberg exchange parameters. These parameters were passed to ALPS thus completing the chain ”crystal structure -⟩ one-electron Hamiltonian -⟩ model parameters -⟩ megnetic susceptibility”.

Data representation in the Molpro quantum chemistry package

Peter Knowles
Cardiff University, UK, United Kingdom

Abstract

The Molpro package (http://www.molpro.net), which is focused on ab initio electronic structure computations for small and medium-sized molecules, contains several facilities for the import and export of portable structured data. Export of molecular geometries and wavefunction data follows an extended CML format, and is augmented by a fully-tagged transcript of an entire job. Internally, the program makes use of a xml-expressed library of basis sets and pseudopotentials that is accessible through interactive documentation, and that is capable of transformation to other formats. These features will be demonstrated through a number of examples, which will then form the basis for a discussion of outstanding and difficult issues, and of the potential for interfacing to other codes and representation schemes.

A common format for Quantum Chemistry

Elda Rossi
CINECA, Italy

Abstract

A Common Format for Quantum Chemistry has been designed and implemented. It responds to the requirement of communication between different QC programs and aims at enhancing code interoperability. A general discussion about a possible model for data organization in the QC domain is reported: small data describing geometry, basis set and symmetry are organized within an XML based format (QC-ML), while large binary data describing integrals and coefficients are organized within an HDF5 based format (Q5COST). Some applications that use the proposed format for running a complex chain of heterogeneous programs, both general purpose and home made, will be presented as well. Last, we will discuss a possible follow up of this activity in terms of workflow and distributed computations (Grids and Web Services).

This activity has been carried out within the COST in Chemistry D23 project ”MetaChema”, in the Working Group ”A meta-laboratory for code integration in ab-initio methods”.

Building an Infrastructure for Quantum Chemistry: Data Sharing and Graphical User Interfaces

Sherwood Paul
Daresbury Laboratory, UK, United Kingdom
Coauthor: Phil Couch

Abstract

We will discuss the work that has been carried out under the CCP1 (Collaborative Computational Project No. 1) with the objective improving interoperability between quantum chemical codes, and providing common tools such as graphical interfaces. I will discuss the issues that have arisen in the consultation processes and discuss possible ways of progressing further the definition of standards for data exchange. I will describe an open source project which aims to provide a common user environment to a number of QM and other modelling codes, and which is being used as prototype in exploring some of the data exchange issues.

Material leading to discussion: Data markup hierarchies and interoperation

Peter Murray-Rust
Unilever Ctr for Mol. Informatics, U. of Cambridge, United Kingdom

Abstract

I would like to give an overview of markup and to review current approaches. My current interpretation is very roughly that there is a rough hierarchy - content+syntax, dictionaries, semantics.

CML tackles content+syntax and provides XSD-like validation (there are a few validation extensions). CML aims to:

- provide unique labels for agreed concepts usable in a wide range of domains
- provide validation
- provide common programmatics functionality
- act as a program- and laboratory- independent nucleus on which others can build.

There seem to be the following types of markup:

- content extensions because the concept is not and cannot be realised in CML. An obvious example is pseudopotential (though not basisSet, which CML supports).
- Program-specific markup (e.g. GAMESS). In CML-language this is a mixture of content and dictionary. It looks as if it can be automatically transformed to CML and a dictionary.
- semantic languages, such as Agent-X, dREL (IUCr), OMDOC, and unstructured RDF. CML itself is neutral to these and can be used by any.

An Introduction to the Use of XMLDIR and QuickSchema

Michael Summers
Oak Ridge National Laboratory, USA, United States

Abstract

XMLDIR has been developed as a common IO subsystem for a family of scientific codes. Its development started with an initial system and continues through incremental refinements based on experience gained by incorporating XMLDIR within existing codes. This experience has provided us with insights into the techincal and organization requirements of such a common IO susbsystem. These insights include an understanding of:

- 1. what new users need to know and do as they integrate XMLDIR into their codes, and
- 2. the need for an easy to use, web-based, collaborative, schema development tool.

This talk will provide a quickstart tutorial for the XMLDIR system and an associated demonstration of a schema development tool.

Research sponsored by the Laboratory Research and Development Program of ORNL, managed by UT-Battelle, LLC for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

XML and the Vienna Ab-initio Simulation Package (VASP)

Orest Dubay
Univ. of Vienna, Austria

Abstract

Our experience shows that a XML based format is a very successful concept in VASP, though it has also some limitations. VASP uses a XML-based output format for more than two years. As a prove of the concept, XML was also used for creation of batch-jobs starting multiple VASP calculations. Our initial goals, design decisions and achievements will be discussed to show the strengths as well as some shortcomings related to the use of XML in VASP.

The VASP XML output can be processed by a tool called ”p4vasp” which will be presented both from the user and the developer perspective. P4vasp can create plots of various quantities (e.g. the density of states and the band-structure), show iso-surfaces, manipulate structures and create simulated scanning tunneling microscopy images. P4vasp is very modular, it is implemented in c++ and python and it can be used as a library in simple python scripts.

At the end we will introduce our vision of the sharing and propose a way how to assemble a data-sharing system from the available open-source technologies.

Information Exchange in Computational Chemistry and Materials Physics - AgentX

Phil Couch
CCLRC-Daresbury Laboratory, United Kingdom
Coauthors: Rob Allan, Paul Sherwood, Peter Knowles

Abstract

Increasingly, solving complex scientific problems requires the use of more than one application cooperatively. Considerable effort has been invested in developing general tools that can be used to specify and execute computational workflows that address such problems. However, despite recent advances in this area, it remains difficult to exchange information between applications, principally due to a lack of data standards.

The problem of information exchange derives, in part, from a difficulty in finding the context or meaning of data represented in documents. This can be addressed through the development of common representations for computational data. A common data model specifies how data should be structured and described according to its context. Tools developed to work with data that conform to this model can form a common component of applications exchanging information. The problem can also be addressed by developing standards that can be used to specify how to locate data with a particular context in a document. The AgentX framework is being developed to manage this task. AgentX abstracts away from the format of the data, resulting in the ability to work transparently with data conforming to different standards. The user is not required to understand the underlying data format. AgentX takes the form of a library, presenting a simple interface and being accessible via wrappers to applications written in C, Python, Perl and Fortran.

The general principles of the AgentX framework will be discussed, along with some current applications in the computational domain.

Evolutionary Construction of Higher-level Constraints over an XML Language; Formalizing Informal Semantics

Toby White
Dept. of Earth Sciences, Univ. of Cambridge, United Kingdom
Coauthor: R. Bruin

Abstract

Within the eMinerals project, we have access to a number of computational chemistry codes; at different levels of theory, and with different purposes; which have in common the notion of simulating the interactions of a system of atoms. We have worked to give these codes CML output, with the initial aim of facilitating the tasks of data interchange. In addition, we have developed visualization tools, based on XSLT, which present the output of the codes in a fashion useful to the simulation scientist. These tools are designed to work agnostically of the code of origin; so the same visual output can be seen from any code which outputs correctly organized

CML. The development and refinement of these visualization tools has, however, highlighted the existence of informal semantics above and beyond the mere syntactical requirements of CML, and has forced us to address these in increasingly formal ways. The specification of these semantics, which effectively subsets and constrains CML further, is of wider applicability than mere visualization.

This talk will discuss the use of XSLT as a transform language for CML, and demonstrate the use of the visualization tools. From this, a wider theme will emerge about the necessity and utility of constraints beyond the syntactical validitiy of CML.

CCPN - automatic code generation from UML data models

Rasmus Fogh
University of Cambridge, United Kingdom
Coauthors: Boucher, W., Vranken, W., Stevens, T.J., Pajon, A., Ionides, J., Henrick, K., Laue, E.D.

Abstract

Software interoperability, data exchange and data harvesting require a data standard that is comprehensive, general, and covers intermediate as well as final results. For practical use it must be precisely defined, easy to validate against, and require few resources to maintain. To become widely adopted it must be attractive to programmers with widely different tastes.

CCPN presents the Memops data modeling framework, developed as part of our work on data standards and software integration for macromolecular NMR spectroscopy, as our solution to this problem. Memops begins with an abstract, implementation-independent data model to be written in UML (unified modeling language). Automatic code generation then produces fully functioning data access implementations for a variety of languages (Python, Java, C/C++, Perl) and storage implementations (XML file and relational database), directly from the abstract model. The autogenerated libraries include object-oriented API implementations, I/O mappings and I/O code (for files) or persistence layers (for databases), XML and database schemas, and documentation. All code works seamlessly together, so that e.g. data loading is triggered automatically when the data are needed. Work on client/server support, transactions/rollback and access control is in progress. The API code verifies the validity of all input data according to the constraints of the model; arbitrarily complex constraints can be entered during of the modeling process. A notifier/listener system is in place to trigger external events when the data change. The model is organised in separate packages, making it possible to cover a wide area of data while allowing each application to use only the relevant parts of the model.

Handling of large datasets in Quantum Chemistry

Antonio Monari
Universita di Bologna Italy

Coauthor: S. Evangelisti

Abstract

Our group has been involved in the development of a common format for code interoperability and communication in the field of Quatum Chemistry. Two libraries have been developed, for the treatment of "small" and "large" data sets, respectively. In particular, we have focused our work on the problem of "large" (binary) data, that represent a peculiarity of QC. We have implemented developed a FORTRAN library based on the HDF5 format (Q5COST), that permits data transfer between the programs that produce one and two-electron integrals (at the moment, DALTON and MOLCAS), and chains for the post-SCF treatment (CI or PT algorithms developed in Toulouse and Ferrara). The use of HDF5 has shown some important advantages: high efficiency for I/O operations on large binary files, independence from the architecture of the resulting files. At the same time, the choice of FORTRAN makes the library of easy use within the community of QC program developers.

Input handling in CP2K

Fawzi Roberto Mohamed

Scuola Normale Superiore, Pisa, Italy

Coauthors: Teodoro Laino, Joost VadeVondele

Abstract

The f90 opensource CP2K project http://cp2k.berlios.de has just rewritten the input. The new input structure has been inspired by XML, and is described in a declarative way. This enables the automatic generation of an always up-to-date description of the input, and the automatic handling of the input. Along with the documentation, the usefulness of our approach has been demonstrated by the ability automatically generate inputs (used in montecarlo, path integral,...).

Participant List

Osvaldo Gervasi (osvaldo@unipg.it)
University of Perugia, Dept. of Maths and Comp Sci Italy

Rasmus Fogh (r.h.fogh@bioc.cam.ac.uk)
University of Cambridge United Kingdom

Antonio Monari (amonari@fci.unibo.it)
Universita' di Bologna Italy

Thomas Schulthess (schulthesstc@ornl.gov)

Oak Ridge National Laboratory United States

Alberto Garcia (wdpgaara@lg.ehu.es)
Universidad del Pais Vasco, Bilbao Spain

Philip Couch (p.a.couch@dl.ac.uk)
CCLRC United Kingdom

Walter Temmerman (W.M.Temmerman@dl.ac.uk)
Daresbury United Kingdom

Martin Lueders (m.lueders@dl.ac.uk)
Daresbury Laboratory United Kingdom

Fawzi Roberto Mohamed (fawzi@gmx.ch)
Scuola Normale Superiore, Pisa Italy

Markus Holzmann (markus@lptl.jussieu.fr)
LPTL, Jussieu, Paris France

Jon Wakelin (Jon.Wakelin@bristol.ac.uk)
University of Bristol, UK United Kingdom

Xavier Gonze (gonze@pcpm.ucl.ac.be)
Universite Catholique de Louvain Belgium

Sherwood Paul (p.sherwood@dl.ac.uk)
Daresbury Laboratory, UK United Kingdom

Paolo Giannozzi (p.giannozzi@sns.it)
Scuola Normale Superiore di Pisa Italy

Javier Junquera (javier.junquera@unican.es)
Univ. Cantabria, Spain Spain

Peter Knowles (KnowlesPJ@Cardiff.ac.uk)
Cardiff University, UK United Kingdom

Peter Murray-Rust (pm286@cam.ac.uk)
Unilever Ctr for Mol. Informatics, U. of Cambridge United Kingdom

Francois Gygi (fgygi@ucdavis.edu)
University of California, Davis United States

Kim Baldridge (kimb@oci.unizh.ch)
Uni Zurich, Organic Chemistry Institute Switzerland

Toby White (tow21@cam.ac.uk)
Dept. of Earth Sciences, Univ. of Cambridge United Kingdom

Richard Bruin (rbru03@esc.cam.ac.uk)
Dept. of Earth Sciences, Univ. of Cambridge United Kingdom

Matthias Troyer (troyer@itp.phys.ethz.ch)
Theoretische Physik, ETH Zü rich Switzerland

Konrad Hinsen (khinsen@cea.fr)
Laboratoire Lé on Brillouin (CEA-CNRS) France

Stefano Evangelisti (stefano@irsamc.ups-tlse.fr)
Universite Paul Sabatier France

Elda Rossi (e.rossi@cineca.it)
CINECA Italy

Jeongnim Kim (jnkim@ncsa.uiuc.edu)
NCSA United States

Orest Dubay (orest.dubay@univie.ac.at)
Univ. of Vienna Austria

Daniel Wilson (wilson@kristall.uni-frankfurt.de)
Univ. of Frankfurt Germany

Michael Summers (summersms@ornl.gov)
Oak Ridge National Laboratory, USA United States

Anton Kozhevnikov (anton@imp.uran.ru)
Russian Acad. Sciences, Russia Russian Federation

3.3 ESF Psi-k Programme Workshop/Conference Announcements

3.3.1 CECAM-Psi-k Workshop on "Catalysis from First Principles"

September 11 - 14, 2006

CECAM, Lyon, France

A limited number of spaces are still available for participants at this joint CECAM - Psi-k workshop being organised by Angelos Michaelides, Matthias Scheffler, Karsten Reuter, Jens Norskov and Juergen Hafner.

This meeting will be the fifth in the "Catalysis from first Principles" series, and will follow successful workshops in Magleas, Denmark (1999 and 2004), Lyon (2000) and Vienna (2002).

Invited Speakers include: Frank Abild-Pedersen, Jesper Andersen, Thomas Bligaard, Charles T. Campbell, Giancarlo Cicero, Michel Daage, Olaf Deutschmann, André Fielicke, Axel Gross, Peijun Hu, Stephen Jenkins, Dieter M. Kolb, Eric McFarland, Florian Mittendorfer, Joachim Paier, Thomas Risse, Jutta Rogal, Jens Rostrup-Nielsen, Joachim Sauer, Philippe Sautet, William F. Schneider, and W. Henry Weinberg.

For more information, including registration details see

http://www.fhi-berlin.mpg.de/th/Meetings/C1P2006/index.html

or

http://www.cecam.fr

The deadline for applications is May 31st, 2006. Accepted participants will be notified in early June.

Dr Angelos Michaelides
Fritz-Haber-Institut der Max-Planck-Gesellschaft
Faradayweg 4-6
D-14195 Berlin
Germany

Phone: +49 30 8413 4801
Fax: +49 30 8413 4701
e-mail: michaeli@fhi-berlin.mpg.de

3.3.2 KKR Workshop Announcement:

"Recent Developments and Applications of the Multiple-Scattering approach to 'First-Principles' Electronic Structure Calculations"

Location: Burwalls, Bristol, United Kingdom

Dates: October 20-22, 2006

Sponsors: Psi-k Network (ESF) and CCP9 (EPSRC)

Organizers: H. Ebert, B. L. Gyorffy, W. M. Temmerman

Local Organizers: J. F. Annett, B. L. Gyorffy, D. A. Rowlands

Confirmed List of Invited Speakers:

Igor Abrikosov (Linkoeping) "*Core Level Spectroscopy in Alloys*"

Gary Batt (Bristol) "*Fermi Surfaces of Random Alloys*"

Ezio Bruno (Messina) "*First-principles Calculations of Phase Diagrams in Metallic Alloys through the Charge Excess Functional - Quantum Monte Carlo Method*"

Hubert Ebert (Munich) "*Combination of the LDA+U and DMFT methods with KKR*"

Aurthur Ernst (Halle) "*GW with KKR*"

Werner Hofer (Liverpool) "*STM and KKR*"

Diemo Kodderitzsch (Munich) "*An Efficient and Fully Relativistic Implementation of the KKR-NLCPA making use of symmetry*"

Ingrid Mertig (Halle) *title to be confirmed*

Derwyn Rowlands (Bristol) "*The Korringa-Kohn-Rostoker Nonlocal Coherent Potential Approximation (KKR-NLCPA)*"

Julie Staunton (Warwick) "*SIC and DLM*"

Valery Stepanyuk (Halle) "*Quantum Resonators on Metal Surfaces*"

Dzidka Szotek (Daresbury) "*Gaps and SIC*"

Laszlo Szunyogh (Budapest) "*Kondo Impurity near a Surface*"

Walter Temmerman (Daresbury) *Valency and SIC*

Paul Tulip (Warwick) "*First-Principles Spectral Function in the KKR-NLCPA*"

Balazs Ujfalussy (Budapest) "*Semi-infinite KKR*"

Levente Vitos (Stockholm) "*The Exact Muffin-Tin Orbitals-CPA Method and Applications*"

Herman Winter (Karlsruhe) "*Calculation of Correlation Functions using the Screened KKR*"

Invited Speakers to be confirmed:

Jurgen Braun (Munich) "*Calculation of Photoemission Spectra on a basis of a combination of the DMFT and KKR methods*"

Peter Dederichs (Julich) "*Magnetic Semiconductors*"

Bence Lanzerovits (Budapest) "*Quantum Corrals*"

Martin Lueders (Daresbury) : "*Local SIC*"

Sergy Mankovsky (Munich) "*Spin and Orbital High-Field Susceptibiblity of Ferromagnetic Alloys calculated using the SPR-KKR*"

Jan Minar (Munich) "*Magnetic Properties of Deposited Transition Metal Clusters*"

Malcolm Stocks (Oak Ridge) "*LSMS*"

Laszlo Udvardi (Budapest) "*Relativistic exchange interactions*"

Andras Vernes (Vienna) "*Pump-Probe Calculations using KKR*"

Peter Weinberger (Vienna) "*Kubo Formula and KKR*"

Rudi Zeller (Julich) "*The Lloyd Formula*"

We have funds to cover local expenses for about 40 people, including the invited speakers, however we hope that the participants will cover their own travel expenses to Bristol. Please email d.a.rowlands@bristol.ac.uk if you are interested in attending.

3.3.3 Workshop on "Models and Theory for Molecular Magnetism"

CECAM, Lyon, France

July 18 2006 to July 21 2006

sponsored by: Psi-k, CECAM and MagmaNet

Jens Kortus, TU Bergakademie Freiberg, Germany

Carlo Massobrio, IPCMS, Strasbourg, France

Eliseo Ruiz, Univ. de Barcelona, Spain

Mark Pederson, NRL, United States

http://www.cecam.fr

The progress in research on molecular magnetism is driven by advances in chemical synthesis of the materials and ingenious experiments. The advances in the capability to predict properties from first-principles calculations gives hope for an rational design of magnetic molecular materials. This workshop brings together leading theoretical groups in order to define long term prospects and challenges for future research in the field of molecular magnetism.

For more details visit `http://www.cecam.fr`.

Registration:

There is no registration fee. Registration is possible through the CECAM webpage `http://www.cecam.fr`.

The deadline is 01.06. 2006.

The number of participants is limited.

3.3.4 Psi-k/COST Workshop on "Multiscale Modeling of Extended Defects and Phase Transformations at Material Interfaces"

Wrocław, Poland

September 24–26, 2006

Sponsors: Psi-k, COST Action P19

Organizers:
Adam Kiejna, University of Wrocław, Wrocław, PL
Mojmir Šob, Masaryk University, Brno, CZ

http://www.ifd.uni.wroc.pl/mmds-wroclaw/

The workshop will be hosted by the University of Wrocław, Poland, for three full days (Sunday – Tuesday), Sept. 24-26, 2006. The workshop is supported by the ESF Programme Psi-k "Towards Atomistic Materials Design", and the ESF COST Action P19 "Multiscale Modeling of Materials", and is a satelite meeting to the MMM2006 conference (http://www.MMM2006.org) to be held Sept.18-22, 2006 in Freiburg, DE .

Overview

Exploring connections between macroscopic characteristics of materials and their microscopic structure in atomic scale is an important topic in contemporary materials science and engineering. The aim of the workshop is to bring together distinguished representatives of physics, chemistry, materials science, and metallurgy communities to present and discuss state-of-the-art developments and the perspectives of theory, techniques, and applications, in multiscale modeling of cohesion and structure of extended defects in materials and their interfaces, fracture mechanics, phase transformations and chemical reactions at materials interfaces, micromagnetism, and polymer processes. The workshop is open to all scientists and students working in the field of modeling of materials.

Programme Advisory Board

M. Alatalo (Lappeenranta, FI)
G. Courbebaisse (Lyon, FR)
H. Dreysse (Strasbourg, FR)
J. Fidler (Vienna, AT)
M. W. Finnis (London, UK)
P. Gumbsch (Freiburg, DE)
J. Hafner (Vienna, AT)
B. Johansson (Stockholm, SE)
K. J. Kurzydłowski (Warsaw, PL)
M. Scheffler (Berlin, DE)

During three days of the workshop there will be about 20 invited talks (50 minutes) each including tutorial introduction, and several selected short presentations (15 min.) of younger researchers. There will be room for 20 posters. Contributions from the field of multiscale modeling of materials are invited. In total we expect about 60 participants.

Invited speakers

Igor Abrikosov (Linköping, SE)
Mikko Alava (Helsinki, FI)
Roy Chantrell (York, UK)
Guy Courbebaisse (Lyon, FR)
Gabor Csanyi (Cambridge, UK)
Christian Elsässer (Freiburg, DE)
Yuan P. Feng (Singapore)
Jürgen Hafner (Vienna, AT)
Takayuki Kitamura (Kyoto, JP)
Stefan Müller (Erlangen, DE)
Jörg Neugebauer (Düsseldorf, DE)
Risto M. Nieminen (Helsinki, FI)
Vaclav Paidar (Prague, CZ)
Karsten Reuter (Berlin, DE)
Dieter Suess (Vienna, AT)
Adrian P. Sutton (London, UK)
Vasyl Tokar (Strasbourg, FR)
Göran Wahnström (Gothenburg, SE)
François Willaime (Saclay, FR)
Dieter Wolf (Idaho Falls, USA)
Sidney Yip (Cambridge, USA)

Registration

The registration fee for the workshop is EUR 80 and includes coffee/tea, lunches, conference dinner, and book of abstracts. Arrival of participants is expected on Saturday (Sept. 23) and departure on Wednesday (Sept. 27).

Deadline for abstracts submission is June 15, 2006.
Deadline for registration is July 1, 2006.

Further information

Adam Kiejna / Elwira Wachowicz
Institute of Experimental Physics
University of Wrocław
50-204 Wrocław
Poland
Phone: +48 (0) 71 3759266
Fax: +48 (0) 71 3287365
E-mail: elwira@ifd.uni.wroc.pl
Webpage: http://www.ifd.uni.wroc.pl/mmds-wroclaw/

3.3.5 Tutorial on "Simulating matter at the nano-scale using density-functional theory, pseudopotentials and plane waves"

CECAM, Lyon

November 6-10, 2006

Sponsors: CECAM, MolSimu, Psi-k

Organizers:
Paolo Giannozzi, SNS Pisa and Democritos Trieste
Xavier Blase, Université Lyon 1 and CNRS
Ralph Gebauer, ICTP and Democritos Trieste

http://www.cecam.fr

This tutorial is aimed at students and young researchers who need an introduction to the field of electronic structure computations. It is also directed to non-specialists (e.g. experimentalists) who need to use the results of computer simulations for their work.

The tutorial will consist in morning lectures, followed by afternoon practical hand-on sessions. In the lectures, emphasis will be put on the fundamental concepts, illustrated by a variety of examples showing the merits, but also the limitations, of the various DFT implementations. In addition to standard ground state properties (equilibrium structure, cohesive energy, etc.) and Kohn-Sham orbitals analysis, an introduction to modern linear response theories (dielectric response, vibrational properties) will be provided. Finally, the concepts and tools of molecular dynamics (Verlet algorithm, thermostats, etc.) will be presented. In the hands-on sessions, examples of practical applications will be shown, using the Quantum-ESPRESSO distribution as computational tool.

The number of participants is limited to 30.

Some background in condensed-matter physics or theoretical chemistry, and a basic knowledge of Unix (Linux), are required. Cecam and MolSimu will provide funding covering travel and living expenses for eligible participants. Interested people should apply via the web site `http://www.cecam.fr` (select *Tutorials* in the *Activities* menu; to apply please require a user and a password if you do not have any, and check that your application is "submitted", not just "open"). Notifications of acceptance will be sent starting in July. It will still be possible to apply until all slots are filled.

4 General Workshop/Conference Announcements

4.1 International School on the Fundamentals of Nanoelectronics

August 27 - September 1, 2006 - Lake Balaton, Hungary

The EU Network "Fundamentals of Nanoelectronics" is hosting an International School for young researchers in the week 27 August to 1 September, 2006. The venue is Lake Balaton, the largest lake in Europe, not far from Budapest, Hungary. We are looking forward to some engaging lectures on the top issues in Nanoelectronics, in the relaxed environment of what is called the "Central European Mediterranean".

Lecturers include

L. Vandersypen, Delft, "Spin Based Quantum Computing"
C. Schoenenberger, Basel, "Electrical Transport in Carbon Nanotubes"
J. van Ruitenbeek, Leiden, "Atomic and Molecular Conductors"
V. Falko, Lancaster, "Graphite Monolayers"
K. Richter, Regensburg, "Semiclassical Methods in Quantum Transport"
G. Zarand, Budapest, "Ferromagnetic Semiconductors"
E. Sukhorukov, Geneva, "Quantum Detectors"
M. Governale, Bochum, "Quantum Pumps"

For more information, including a registration form, see

http://gawain.elte.hu/mcrtn/

The school is open for all nationalities. Please note the deadline of June 20, 2006. Because of the limited capacity at the venue we encourage early applications.

Jozsef Cserti & Carlo Beenakker
Program Committee

4.2 LAW3M 2007

First Announcement

LATIN AMERICAN WORKSHOP ON MAGNETISM AND MAGNETIC MATERIALS AND THEIR APPLICATIONS (LAW3M 2007)

Rio de Janeiro, Brazil
12-16 August, 2007
http://www.law3m.org

GENERAL INFORMATION

Venue

The LAW3M Conference will be held at a hotel in the tourist district of Rio, close to the famous beaches of Copacabana and Ipanema.

Aim of the Conference

This meeting will continue the tradition of the previous conferences in La Habana (1991), Guanajuato (1993), Merida (1995), São Paulo (1998), Bariloche (2001), Chihuahua (2003) and Reñaca (2005). The purpose of the Workshop is to stimulate the exchanges between specialists from different parts of the world and the magnetism community in Latin America.

In the week preceding the Workshop, it will be held in Rio the VI Brazilian School of Magnetism (VIEBM). We hope that many students from different Latin American countries will be able to attend both the School and the Workshop.

Topics

All topics in magnetism are acceptable at LAW3M. Contributions in the following ones are expected:

Giant magnetoresistive and giant magnetoimpedance materials
Hard magnetic materials and their applications
Imaging and probe techniques
Magnetic effects on biological systems
Magnetic fluids
Magnetic materials and advanced characterization
Magnetic materials in high magnetic fields
Magnetic recording materials
Magnetocaloric, magnetostrictive and ferromagnetic shape memory materials
Micromagnetism, magnetization processes and magnetic viscosity
Molecular magnetism

Nanostructures, surfaces and interfaces
Numerical modeling, devices and machines
Particles and nanoparticles
Sensors and micro-devices
Soft magnetic materials and their applications
Spin electronics, spin transport phenomena and magnetic semiconductors
Strongly correlated systems
Superconductivity

Sessions

The Conference will have plenary sessions devoted to invited lectures and to short contributed oral presentations, as well as poster sessions.

Working language

The working language of the Workshop is English.

Organizing Committee

A. P. Guimarães, Chair
J. P. Sinnecker, Secretary
J. D'Albuquerque e Castro, Head, Program Committee
A. Azevedo
H. L. Barros
R. Iglesias
M. Knobel
W. Macedo
F. P. Missel
H. R. Rechenberg
R. L. Sommer

Local Committee

M. Bahiana
M. A. Novak
N. A. Oliveira
R. L. Sommer
R. B. Scorzelli
P. Venezuela

Abstracts

The instructions for the preparation and submission of abstracts will be available in the forthcoming circulars.

Pre-Registration

Those interested in receiving the next circulars should fill the pre registration form at the conference homepage at http://www.law3m.org.

Accommodation

There is an ample choice of Hotel accommodations around the Conference venue. Details will be available at the homepage.

Transportation

Rio de Janeiro is served by most major airlines.

Passport and Visa Requirements

Most participants will only need a valid passport. However, a tourist visa will be required from citizens of some countries. In this case, the visa can be obtained from the Brazilian Consulate. Participants should ask their travel agents whether or not nationals from their country require a visa.

Important Dates

Those will be given in the Call for Papers circular.

Contact

secretary@law3m.org

We look forward to seeing you in Rio in 2007.

A. P. Guimarães

4.3 International Symposium on Materials Issues in Hydrogen Production and Storage

August 20-25, 2006

University of California, Santa Barbara CA 93106

Organized by

C. G. Van de Walle (UCSB), W. Goodman (Texas A & M), and J. Eckert (UCSB & LANL)

The International Center for Materials Research at the University of California, Santa Barbara will host an International Symposium to address materials problems in two major areas of basic research aimed at utilization of hydrogen as a fuel, namely in the production and storage of hydrogen. The program will consist of invited talks by leaders in the field on forefront research (both theoretical and experimental) in hydrogen production and storage. Contributed papers are solicited. A limited amount of financial support is available (application deadline: May 17).

For details, see

http://www.icmr.ucsb.edu/programs/HydrogenSymposium.html/

For more information, contact:

Jennifer Ybarra
E-mail: Ybarra@icmr.ucsb.edu
Phone: 805-893-5850
Fax: 805-893-8797

4.4 KINKEN-WAKATE 2006: 3rd Materials Science School for Young Scientists

"Physics and Applications of Advanced Magnetic Materials"

Organized by

International Frontier Center for Advanced Materials (IFCAM) Institute for Materials Research, Tohoku University & The 21st Century COE Program "International Center for Research and Education for Materials"

Date: 2006 August 26th (Sat.) - 28th (Mon.)
Venue: "Hotel Iwanuma-ya", Akiu-spa, Sendai, Japan
`http://www.iwanumaya.co.jp/e_web/index.html`

We would like to bring your attention to an upcoming ICM2006' s satellite meeting, KINKEN-WAKATE 2006, an international summer school for young scientists majoring materials science to be held in Sendai, Japan from August 26 to 28 right after ICM2006. In this school, physics and applications of magnetism are specially focused.

This school includes invited lectures, and contributed poster presentations by young scientists. Ph. D. students and PostDoc are welcome to participate.

Invited Lecturers:

I. Zutic (State University of New York)
W. Wulfhekel (Universitaet Karlsruhe)
A. Hoffmann (Argonne National Laboratory)
T. Kimura (Bell Labs, Lucent technologies)
K. Hono (National Institute for Materials Science)
Y. Ando (Tohoku University)
J. Nitta (Tohoku University)
T. Tohyama (Tohoku University)

Lectures are given in English.

Deadline: June 15 (both registration and abstract).

School Contact: IFCAM Office, ifcam@imr.tohoku.ac.jp

ICM2006 Conference Secretariat
FAX +81-6-6456-4105
E-mail icm2006@jtbcom.co.jp

Please see the following URL for details:

http://www.ifcam.imr.tohoku.ac.jp/School2006/

Prof. Masashi Kawasaki
General Chair of KINKEN-WAKATE 2006
Institute for Materials Research, Tohoku University

4.5 Actinides Symposium at the Fall Meeting of the MRS

November 27 - December 1, 2006

Boston, MA, USA

Symposium OO: "Actinides – Basic Science, Applications, and Technology"

There will be an Actinides Symposium at the Fall Meeting of the MRS in Boston, MA, USA, during November 27 - December 1, 2006. Please see below the Call for Papers. For additional information, please visit the web-site at

http://www.mrs.org/

There will also be tutorials on Sunday by John Sarrao (LANL), Adam Schwartz (LLNL), and Heino Nitsche (LBL/UC-Berkeley).

Abstract Deadline: June 20, 2006

Actinides play an important role in modern society. Though useful in some respects, they can also pose a hazard and must be controlled and well understood. But understanding these materials has been difficult because of their complex electronic structures that challenge theorists and modelers, and complex phase diagrams and phase transformations that challenge experimentalists. Furthermore, many actinide elements are relatively new materials; and their aging behavior is not known, particularly with regard to the effects of self irradiation and the accumulation of radioactive decay products. A goal of this symposium is to bring together researchers studying basic actinide science and those focused on developing technological solutions to the challenges actinides pose in our society. Both experimental and computational studies will be included in the symposium.

Session Topics will include:

Advanced characterization tools (including nuclear magnetic resonance)
Waste form materials science
Materials for actinide detection
Aging of actinide materials
Electronic and magnetic properties
Fundamental physical properties, including metallurgy
Behavior under extreme conditions, including high pressure
Actinide compounds
Separation science
Molecular/solution chemistry

Coordination chemistry
Superconducting actinide materials

Joint Sessions Joint sessions with Symposia MM: Magnetic Resonance in Material Science, and NN: Scientific Basis for Nuclear Waste Management XXX, are under consideration.

A tutorial complementing this symposium is tentatively planned. Further information will be included in the program that will be available in September.

Invited Speakers

Invited speakers (partial list) include: Nathalie Baclet (Commissariat a l'Energie Atomique-Ctr. de Valduc, France), Lynn Boatner (Oak Ridge National Lab), Nerine Cherepy (Lawrence Livermore National Lab), Herman Cho (Pacific Northwest National Lab), Peter Dorhout (Colorado State Univ.), Dan Farber (Lawrence Livermore National Lab), Ian Farnan (Univ. of Cambridge, United Kingdom), John Gibson (Oak Ridge National Lab), Anne E.V. Gorden (Auburn Univ.), Thomas Gouder (Inst. for Transuranium Elements, Karlsruhe, Germany), Richard Haire (Oak Ridge National Lab), Jason Lashley (Los Alamos National Lab), Alexander Lichtenstein (Univ. of Hamburg, Germany), Naoto Metoki (Japan Atomic Energy Research Inst., Japan), Peter M. Oppeneer (Uppsala Univ., Sweden), Anthony Peurrung (Pacific Northwest National Lab), Alexander B. Shick (Inst. of Physics of the Czech Academy of Sciences, Prague), James Smith (Los Alamos National Lab), Lynda Soderholm (Argonne National Lab), Joe Thompson (Los Alamos National Lab), Franck Wastin (Inst. for Transuranium Elements, Karlsruhe, Germany), and Bill Weber (Pacific Northwest National Lab).

Symposium Organizers

Kerri Blobaum
Lawrence Livermore National Laboratory
E-mail: blobaum1@llnl.gov

Elaine Chandler
Lawrence Berkeley National Laboratory
E-mail: eachandler@lbl.gov

Ladislav Havela
Charles University
E-mail: lhavela@seznam.cz

M. Brian Maple
University of California-San Diego
E-mail: mbmaple@ucsd.edu

Mary Neu
Los Alamos National Laboratory
E-mail: mneu@lanl.gov

The abstract submission site will open on May 20th. Please visit the `http://www.mrs.org/s_mrs/sec_mtgdetail.asp?CID=6073&DID=167209>MRS` web site for more information.

5 General Job Announcements

Postdoctoral Position

Atomic Scale Modelling of Insulators

Technische Universität Chemnitz, Germany

Atomic Scale Modelling is reaching industry! Do you want to apply your knowledge to industrial applications?

The group of Prof. Radehaus has ongoing collaborations with several microelectronics companies. In the framework of these projects we have open postdoc positions in the area of ab initio based computations of semiconductor/insulator interfaces, defect states in insulators, high-k materials and tunneling through MOSFET structures on the basis of TDDFT, GW, etc., methods.

Applicants with good knowledge in simulation techniques, ab initio DFT-like computation and programming abilities in C and FORTRAN, are welcome to apply for the positions. Applications including a CV, a list of publications and at least 2 letters of recommendations should be sent as soon as possible to the address below. The applicants should be able to start not later than the 1st of July 2006.

Prof. Chr. Radehaus
Professor Opto- und Festkörperelektronik
Technische Universität Chemnitz
Fakultät Elektrotechnik und Informationstechnik
09107 Chemnitz
Fax: 0371/531-3004
Mail: opto@etit.tu-chemnitz.de
Homepage: http://www.tu-chemnitz.de/etit/opto/

Postdoctoral Position
University of California, Davis

A postdoctoral position in theoretical condensed matter physics is available immediately at the Physics Department of University of California, Davis.

This project is part of a research program that focuses on the development of a better phenomenological and microscopic understanding of the novel heavy fermion 1-1-5 based superconductors. It involves developing and applying to these materials new methods for calculating electronic properties of strongly correlated systems using combinations of density functional and dynamical mean field based methods, while working in close collaboration with leading experimentalists in this area.

We are looking for an exceptionally able and energetic individual who will join the U C Davis theoretical research group led by Daniel Cox, David Pines, and Sergey Savrasov, which has close ties to the heavy electron experimental groups at UC Irvine, Michigan, UIUC, and Los Alamos National laboratory.

Prospective applicants should hold a PhD or equivalent degree in physics. Experience with density functional and many body calculations, Quantum Monte Carlo, numerical methods and programming using Fortran, Java and/or C++ is highly desired.

Interested candidates should email their resumes and the names of at least two references to Sergey Savrasov at

savrasov@physics.ucdavis.edu

For additional information about the Department of Physics at UC Davis, please visit our web site

http://www.physics.ucdavis.edu.

The University of California is an Affirmative Action, Equal Opportunity Employer

Post-Doctoral Position
Materials Science Institute, University of Dresden, Germany

A Post-Doctoral position is immediately available in the “materials science and nanotechnology” group of the Materials Science Institute of the University of Dresden to perform density-functional theory calculations and first-principles molecular dynamics simulations to investigate the processes of oxidation of PtPd alloys and the catalytic activity of their oxidised surfaces towards the oxidation of carbon compounds. These studies aim at a mechanistic understanding of the catalytic activity of bimetallic alloys and are embedded in existing experimental activities within the group, centred on the biomimetic synthesis and physical characterisation of metallic nanoparticles for catalytic applications. The research work will be performed under the direction of Prof. Wolfgang Pompe within a DFG project in collaboration with the Fraunhofer Institute for Mechanics of Materials, Freiburg.

The position will be initially for two years, but is renewable for a third year. Remuneration will be offered corresponding to the German BAT IIa salary scheme. Candidates are expected to possess a solid background in materials science, physics, chemistry or engineering, computer programming skills, and the ability of working independently and collaborating with other scientists. Existing expertise in the atomistic modelling of materials, DFT-based simulations, solid state physics, or surface chemistry represents a strong advantage. Knowledge of the German language is not necessarily required.

Interested candidates should send their applications including CV, publication list and two recommendation letters, by regular or electronic mail, to:
Prof. Wolfgang Pompe (pompe@tmfs.mpgfk.tu-dresden.de), Institut für Werkstoffwissenschaft, Technische Universität Dresden, Hallwachsstr. 3, 01069 Dresden, Germany.

Ph. D. Position

Fraunhofer Institute for Mechanics of Materials (IWM), Freiburg, Germany

A PhD position is immediately available in the “physical modelling of materials” group at the Fraunhofer IWM to perform density-functional theory calculations and first-principles molecular dynamics simulations to investigate the processes of oxidation of CoCrMo alloys and the chemical activity of their oxidised surfaces. These studies aim at an understanding of the bioactivity and biocompatibility of materials for medical implantations and will contribute towards a detailed knowledge of the complex chemistry at the interface between biomaterials and living tissues. The research work will be performed under the direction of Prof. Peter Gumbsch and Dr. Lucio Colombi Ciacchi within a DFG project in collaboration with the University of Dresden.

Candidates are expected to possess a solid background in materials science, physics, chemistry or engineering. Existing expertise in the atomistic modelling of materials, DFT-based simulations, solid state physics, or surface chemistry represents an advantage. Knowledge of the German language is not required.

Interested candidates should send their applications including CV and academic record, preferably via electronic mail, to Lucio Colombi Ciacchi (lucio@izbs.uni-karlsruhe.de), Fraunhofer Institut für Werkstoffmechanik, Wöhlerstr. 11, 79108 Freiburg, Germany. Tel: +49 (0)761 5142113.

Postdoctoral Position

Université de Bourgogne – CNRS, Dijon, France

Title: Theory of Resonant Photo-Electron Diffraction

A postdoc position in **theoretical solid state physics/quantum chemistry** is open in the physical chemistry department of the Université de Bourgogne - CNRS, Dijon, France. The position is offered for 18 months and the starting date should be within 2006.

The selected candidate will work on the **theory of resonant photo-electron diffraction**. Resonant photo-electron diffraction (RPED) is a new experimental method using synchrotron radiation. Non-resonant PED has been used for decades to probe the electronic and structural properties of surfaces and adsorbates. The new feature is the resonant excitation of the photoelectron by means of synchrotron radiation. It results in a strong enhancement of the signal such that impurities and adsorbates in very low concentration can be studied. This is of great relevance for surface chemistry and catalysis applications.

The theory and computer codes for RPED are being developped in our group in collaboration with groups in Paris (SOLEIL) and Rennes (France). The project has received funding from the new french research agency (ANR).

Candidates must hold a PhD in physics or chemistry and must have a strong background in **electronic structure theory** of atoms, molecules and solids. Working experience on the **theory of X-ray and electron spectroscopies** is greatly appreciated. Candidates should send a curriculum vitae and list of publications to the contact person below. Selection will start immediately and continues until the position is filled.

Contact person:
Dr. Peter Krüger, e-mail: pkruger@u-bourgogne.fr, phone: +33-38039-6155
Laboratoire de Recherches sur la Réactivité des Solides (LRRS)
UMR 5613 Université de Bourgogne - CNRS, B.P. 47870, 21078 Dijon, France

Ph. D. Position

ETH Zürich, Switzerland

We seek a highly motivated PhD candidate, with strong background in chemistry and/or physics. The research project, led jointly by the Quasicrystals and Theoretical Mineral Physics groups at Swiss Federal Institute of Technology (ETH Zurich), will involve computational design and experimental synthesis of novel quasicrystals. This project will involve the use of a novel methodology for crystal structure prediction developed at the Theoretical Mineral Physics group and will likely result in the discovery of several new compounds with unusual structures and properties.

To apply, please send your CV, publication list, and 2 letters of reference to Prof. Artem R. Oganov: a.oganov@mat.ethz.ch.

Two Ph. D. Positions
at the Fritz Haber Institute, Berlin, Germany

The Theory Department of the Fritz Haber Institute of the Max-Planck-Society invites applications for two Ph.D. studentships funded through the newly established Marie Curie early stage training network, MONET: Molecular Networks at Phase Boundaries.

Research in our department is aimed at understanding important phenomena in surface-, materials-, and nano-science. With about 50 scientists from many countries the Theory Department provides a lively and stimulating international atmosphere for students in one of Europe's most vibrant capital cities. For more information of the Theory department see:

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

We are looking for highly qualified students from physics, chemistry, and materials science that hold a Masters Degree (or equivalent) and fulfill the requirements of nationality and residence as outlined on the MONET website:

http://www.sljus.lu.se/monet/index.html

Further details of the proposed PhD projects can also be found at the MONET site.

We will consider applications until the positions are filled. Please send your application by email or regular mail to

Dr Angelos Michaelides
Fritz-Haber-Instituts der MPG
Faradayweg 4 - 6
D-14195 Berlin
Germany

E-Mail: michaeli@fhi-berlin.mpg.de
WWW: http://www.fhi-berlin.mpg.de/th/th.html

Ph. D. and/or Postdoctoral Positions
Institute for Inorganic Chemistry, RWTH Aachen, Germany

Applications are invited for two Ph. D. or PostDoc positions in Computational Materials Science at the Institute for Inorganic Chemistry at the RWTH Aachen, Germany.

The projects concern modelling and simulations in the field of nanostructures: nano-domains in amorphous ceramics, Si and Ge quantum dots, and precipitation of clusters in glasses. The work is highly interdisciplinary and has an international research profile; collaboration are with experimental groups from chemistry, physics, and engineering. The funding of the projects is granted for an initial period of 3-years, but can be extended for up to 6-years.

Successful applicants for a PhD-studentship should have demonstrated their interest for theoretical and computational science. For post-doctoral candidates experiences in the application of DFT methods for extended systems is mandatory.

The positions are open immediately with a mutually agreed starting date. Requests for further information and applications should be sent to

PD Dr. Peter Kroll
Anorganische Chemie, RWTH Aachen, Landoltweg 1
52056 Aachen, Germany E-mail: peter.kroll@ac.rwth-aachen.de.

Postdoctoral Positions for theoretical research on magnetoelectrics

Institut de Ciencia de Materials de Barcelona, Spain
& Universite de Liege, Belgium

Two post-doctoral positions are available, one with Jorge Iñiguez at ICMAB-CSIC in Barcelona (http://www.icmab.es/dmmis/leem/jorge) and one with Philippe Ghosez at ULg in Liege (http://www.phythema.ulg.ac.be/Personnes/ghosez.htm), to conduct theoretical research on magnetoelectric systems.

Research project

The research project concerns the quantum theory and modeling of magnetoelectric materials. It will take place in the context of the MaCoMuFi European STREP project that also involves the leading experimental groups in the field in Europe.

Practical aspects

The initial contract will be for one year starting in September 2006, with possible renewals up to 3 years. One position is in Barcelona and the other in Liege but both persons will have to work in close connection and to collaborate with the experimental groups of the MaCoMuFi project.

Candidates

The candidates should have experience with first-principles computational methods. Previous work on strongly-correlated systems and development of first-principles methods will be highly valued.

Application

Candidates can send (i) a letter of motivation, (ii) a CV and (iii) two recommendation letters to Dr. Jorge Iñiguez (jiniguez@icmab.es) or Prof. Philippe Ghosez (Philippe.Ghosez@ulg.ac.be).

Jorge Iñiguez - Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC, Spain), Laboratory of Electronic Structure of Materials
Philippe Ghosez - Insitut de Physique (Universite de Liege, Belgium), Group of Theoretical Physics of Materials.

Ph.D. Position

Université de Bourgogne – CNRS, Dijon, France

A PhD position is opening in the physical chemistry department of the Université de Bourgogne - CNRS, Dijon, France. The position is offered for three years and the starting date must be between september and november 2006. Applicants must hold a masters degree in physics or chemistry and should have a good knowledge of quantum mechanics and experience in computer programming (Fortran, C).

The subject of the PhD thesis is the **development of computational methods for Resonant Photo-Electron Diffraction** (RPED). Depending on the interests of the candidate, a substantial part of the work may also deal with experimental studies using RPED.

Non-resonant PED has been used for decades to probe the electronic and structural properties of surfaces and adsorbates. The new feature is the resonant excitation of the photo-electron by means of synchrotron radiation. It results in a strong enhancement of the signal such that impurities and adsorbates in very low concentration can be studied. This is of great relevance for surface chemistry and catalysis applications.

Theoretical and computational as well as experimental aspects of RPED are being developped in our group in collaboration with groups in Paris (SOLEIL) and Rennes (France). The project has received funding from the new french research agency (ANR).

Contact person:
Dr. Peter Krüger, e-mail: pkruger@u-bourgogne.fr, phone: +33-38039-6155
Laboratoire de Recherches sur la Réactivité des Solides (LRRS)
UMR 5613 Université de Bourgogne - CNRS, B.P. 47870, 21078 Dijon, France

Postdoctoral Fellow

Computational Chemistry

National Institute for Nanotechnology, Edmonton, Alberta, Canada

We are currently looking for a post-doctoral fellow in computational chemistry. Candidates from physical chemistry/chemical engineering with strong computational background are expected to apply. He/she is required to carry out quantum chemical simulations using various software packages. Some knowledge of zeolitic cluster models, prediction of reaction pathways, and calculation of kinetic and thermodynamic parameters from quantum chemical simulations is required.

The position is based at the National Institute for Nanotechnology (http://www.nint.ca), which is located on the University of Alberta campus in Edmonton, Alberta. The work involves collaboration between NINT and National Center for Upgrading Technology scientists and requires that the successful candidate travel to Devon, Alberta (20 minutes south of Edmonton) on occasion.

Interested candidates should send their CVs to Gino.DiLabio@nrc-cnrc.gc.ca.

Dr. Gino A. DiLabio
National Institute for Nanotechnology
National Research Council
W6-010 ECERF
9107 116th Street
Edmonton, AB
Canada
T6G 2V4

TEL: 1-780-492-8899
FAX: 1-780-492-8632

Ph. D. Position

Max-Planck Institute for Polymer Research
Mainz, Germany

A PhD position is available at the Max-Planck Institute for Polymer Research in Mainz (Germany) within the Marie Curie EuroSim Program: "Host fellowships for Early Stage Research Training (EST)". (see also:

http://www.mc-eurosim.cecam.org/index.php?content=activities/jobOffer)

The subject is the Modeling and Study of the Adsorption of biomolecules on metal surfaces, using different simulation techniques and combinations thereof. The candidate is expected to have a strong background in at least one of the following disciplines; applied mathematics, physics, chemistry. Previous experience with classical or quantum simulations is preferred. For further information please contact:

Luigi Delle Site, e-mail: dellsite@mpip-mainz.mpg.de

Postal address:

Luigi Delle Site
Max-Planck-Institute for Polymer Research
Theory Group
PO Box 3148
D-55021 Mainz,Germany
Phone:+49 (0)6131 379 328
FAX:+49 (0)6131 379 340
`http://www.mpip-mainz.mpg.de/~dellsite/multiscale/`

Post-doctoral Research Fellow

UCL Department of Physics & Astronomy

and London Centre for Nanotechnology (LCN)

Ref: DB/05/06

Modelling Charge Transport in Conducting Polymers and Biological Systems

Applications are invited to work as part of a team including Dr David Bowler, Dr Andrew Horsfield, Prof. Mike Gillan and Prof. Andrew Fisher. This project aims to shed new light on fundamental electronic processes in single molecular systems by the application of state-of-the-art modelling in collaboration with experimental work. We will apply the linear-scaling ab initio code CONQUEST and Correlated Electron-Ion Dynamics formalism (CEID) to systems being investigated experimentally in the IRC at Bristol , Cambridge and UCL. The longer term aim is to create a connected set of related projects which can feed into and support each other.

The objectives will be: to understand the transport properties of molecular wires, poly-rotaxanes (insulated molecular wires) and biomolecules, in particular the conduction mechanisms and the effects of interactions with an environment; to enhance and make available a powerful tool for investigating the properties of semiconducting polymers in complex environments, by implementing mixed basis sets, embedding and CEID into CONQUEST.

The post is for up to two and a half years subject to successful probation. The starting salary will be £24,886 plus £2,400 pa London Allowance. PhD and research experience in Condensed Matter Physics, Materials Science or Quantum Chemistry is required. Previous extensive experience in studying materials properties using quantum mechanical methods and atomistic simulations and ability for scientific programming are essential. The appointee's duties will include a small amount of teaching for the Department.

Enquiries should be addressed to Dr David Bowler (david.bowler@ucl.ac.uk).

Closing date for applications is Friday 9 th June 2006.

HOW TO APPLY

An application form may be obtained from Ms. Denise Ottley, tel. +44 (0)20 7679 8350 or e-mail: d.ottley@ucl.ac.uk. The application form may be also downloaded from:

`http://www.ucl.ac.uk/hr/docs/download_forms/job_app.doc`.

The completed application form, CV and list of publications should be sent strictly by post to: Ms Denise Ottley, Department of Physics and Astronomy, University College London, Gower

Street, London WC1E 6BT, UK.

Closing date for applications is Friday 9 th June 2006.

Please see

http://www.phys.ucl.ac.uk/people/vacancies/Resf39.htm

for person and job specifications.

David Bowler
Department of Physics & Astronomy
University College London
Gower St, London, WC1E 6BT, U.K.

Tel:+44 207 679 7229
Fax:+44 207 679 1360
E-mail: david.bowler@ucl.ac.uk
`http://www.cmmp.ucl.ac.uk/~drb/`

Ph. D. Position

London Centre for Nanotechnology and Department of Physics and Astronomy, University College London

”Developing Mechanisms of Laser-Induced Processes at Surfaces”

A FOUR year fully funded studentship is available to applicants who have been resident in the UK for not less than 3 years and have gained or are expected to gain a first or upper second class MSci degree or equivalent. The studentship is to study towards a doctorate in molecular modeling and material simulation at the London Centre for Nanotechnology under supervision of Prof Alexander Shluger.

This THEORETICAL research project is focused on developing mechanisms of laser-induced processes at surfaces. It is co-funded by Pacific Northwest National Laboratory (PNNL), WA, USA, which will provide an annual 3,000 GBP top-up to the UCL level of studentship (currently 14,000 GBP). Collaboration with the experimental work at PNNL is essential. It will focus on the mechanisms of laser-induced modification of atomic surface structure of oxide nano-particles and on laser-induced electron-transfer between porphyrine molecules and oxide surfaces. Control over surface morphology and chemical functionality is a major challenge in developing novel technologies in chemistry, electronics, and biology and will be addressed in this project via close collaboration between theoretical modeling and experiment. The research will involve learning and developing computational methods of electronic structure calculations, calculations of excited states, and modeling surface structures and reactions. For more information please access www.cmmp.ucl.ac.uk/ kpm/.

Preliminary email applications are encouraged (Prof. Alexander Shluger, a.shluger@ucl.ac.uk). Applicants must send a hard copy of the PhD application form (which can be downloaded from www.ucl.ac.uk) to Prof. A. Shluger, Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK.

Deadline for applications 20 June, 2006.

Postdoctoral Researcher
Hunter College of CUNY (City University of New York)

There is an opening for a postdoctoral researcher in my group at Hunter College of CUNY (City University of New York). The group (PI Neepa Maitra) conducts research in functional development in time-dependent density functional theory, for use in chemistry and in strong-field physics. Experience in density functional theory methods is desirable, although not necessary. This position could be suitable for a person with a PhD in either chemistry or physics. The start date could be as early as September.

Interested parties should send a CV electronically to me at

nmaitra@hunter.cuny.edu

and have three letters of recommendation emailed there.

If preferred, you may send the materials by mail to:

Neepa Maitra Department of Physics and Astronomy
Hunter College of CUNY
695 Park Avenue
New York, NY 10021

Applications will be considered immediately and continue until the position is filled.

FELLOWSHIP FOR DEVELOPMENT OF HYBRID AB INITIO METHODS FOR BIOLOGICAL SYSTEMS AND MATERIAL SCIENCE

C.A.S.P.U.R. & Univ. of Rome ”La Sapienza”, Italy

Theoretical investigation of the electronic properties of biological and condensed matter systems in which electron correlation plays a major role - such as in half-filled-d-shell transition metals (Cr,Fe,Ni,Mo,...) or in excited states - needs the use of very accurate computational methods such as Quantum Monte Carlo (QMC). Interfacing QMC methods with Molecular Mechanics (MM) or Density Functional Theory (DFT) would provide us with the opportunity to study such electronically highly correlated systems in their complex environment.

The present fellowship is focused on the development and implementation of electronic structure software aimed to perform hybrid simulations based on Quantum Monte Carlo. In particular, interfaces with classical force-fields (QMC/MM) and DFT calculations (QMC/DFT) will be realised.

The candidate should hold a PhD in Physics, Chemistry, or related fields. Programming experience on electronic structure software is essential, with preference to Density Functional Theory and Quantum Monte Carlo.

Interested applicants should send a curriculum, a publications list and the names and contact information of two people who can provide a reference.

Contacts:

PhD Simone Meloni (s.meloni@caspur.it), CASPUR
Phone: +39 06 44486711

Prof. Leonardo Guidoni (leonardo.guidoni@uniroma1.it)
Physics Dpt., Univ. of Rome ”La Sapienza”
Phone: +39 06 4991 3314; Web: http://bio.phys.uniroma1.it

A copy of the present announcement is present at

http://www.caspur.it/ilconsorzio/opportunitadilavoro/

Ref:APPMATSCI0506

A Postdoctoral Research Assistant position is available to work on the EPSRC-funded theoretical project "Disorder-Controlled Quantum Transport in Carbon Nanotubes" in the Theoretical Physics research group at the University of Birmingham, UK. This EPSRC-funded project involves collaboration with the experimental group of Professor A Savchenko at the University of Exeter.

Applicants must hold a PhD or equivalent, and should have a strong research and publication record in theoretical condensed-matter physics or a related field. A working-level familiarity with analytic approaches to strongly-correlated systems and/or mesoscopic electronic systems would be advantageous.

Closing date for applications is 26 May 2006 with the position available from 30 June 2006. A full description and an application form (which should be accompanied by three letters of reference) are available at the following link

http://www.personnel.bham.ac.uk/vacancies/furtherParticulars.htm?refNo=43017

Informal enquiries should be e-mailed to Igor Lerner (ivl@th.ph.bham.ac.uk).

Ph. D. Positions
SISSA, Trieste, Italy

Applications are invited for several 3-year PhD positions in Theory and Numerical Simulation of Condensed Matter (CM) at the International School for Advanced Studies (SISSA) in Trieste. The earliest deadline for selection is September 20th, 2006

(`http://www.sissa.it/main/?p=AC_B1_C2&id=152`). Admissions are based

on entrance exams, which will take place in Trieste on October 4th and 5th, 2006 (some travel reimbursement is available). 2006 Courses will begin November 7th, 2006.

Admissions for 2007 will also be possible without sitting the entrance exam, based on purely paper selections (Non-Europeans only) at a later application deadline around March 10, 2007.

The CM curriculum in SISSA involves a strong training in basic many body theory, in numerical simulation of condensed matter, solid state physics, electronic structure and statistical mechanics, as well as a vigorous research activity in a variety of areas as at

http://www.sissa.it/cm

Faculty in condensed-matter theory and simulation sector include: S. Baroni, A. Dal Corso, M. Fabrizio, S. Fantoni, R. Fazio, S. de Gironcoli, G. Santoro, G. Scoles, S. Sorella, E. Tosatti.

The School hosts the DEMOCRITOS National Simulation Center (www.democritos.it) of CNR-INFM whose activities also involve most SISSA CM faculty members, and an additional faculty consisting of F. Becca, S. Cozzini, S. Fabris, and S. Moroni.

Scientific collaboration is lively with other major scientific institutions on the Miramare campus, including the Theoretical Physics Department of Trieste University (http://www-dft.ts.infn.it) and the Abdus Salam International Centre for Theoretical Physics (ICTP) (http://www.ictp.it), both of which host strong CM groups. In addition, the ICTP runs on campus many conferences and schools each year on Condensed Matter related subjects.

Close contacts are entertained with experimental laboratories at the Elettra Synchrotron Light Laboratory and at the TASC/INFM Laboratory in the Trieste Basovizza campus, about 1/2 hour away from Miramare. A small theory group has been recently established in Basovizza under the aegis of DEMOCRITOS, thus providing a rich interdisciplinary scientific and educational playground.

Successful applicants will, irrespective of their nationality, gender, and creed be offered a fellowship that will enable them to pursue a first class PhD under the supervision and in close research contact with the faculty, in a stimulating environment of visiting scientists and postdocs.

All activities of SISSA are conducted in English, no knowledge of Italian is required. SISSA has trained PhDs in Condensed Matter Theory for about 25 years, and past SISSA students hold a very good scientific record. Several of them now occupy important positions worldwide.

Trieste and the Miramare campus offer a site of unique beauty, poised right on the Adriatic seashore but close to the Carso hills (See e.g. http://www.ts.camcom.it/ENGLISH/tourism.htm, http://www.triestetourism.it/).

For further information check www.sissa.it/cm (→ PhD admissions) or contact CM sector secretariat, Ms. Lorena Bencina (bencina@sissa.it).

Three Postdoctoral Positions (A660, A661, A662) in "Mesoscopic Physics and Theory of Nanoelectronic Structures" at Lancaster University, UK

The Physics Department and the Centre for Nanoscale Dynamics and Mathematical Physics at Lancaster University will be filling three postdoctoral positions (RA) funded by the European Commission and EPSRC UK. One of these posts (A660) belongs to the Marie Curie Excellence Team 'NanoElectroPhotonics' led by Dr. H. Schomerus. It will focus on electronic and photonic transport and dynamics in low-dimensional quantum systems. The other two posts are part of the ESF collaborative project 'SpiCo' (A661) and the EU Project 'DynaMax' (A662) led by Prof. V. Falko. These will address theory of quantum transport and dynamics in semiconductor quantum dots and in graphene, and dynamical properties of ferromagnetic nanostructures. Applicants should hold or be close to acquiring a PhD in theoretical condensed-matter physics, quantum optics, quantum dynamics, or a related field. Computational experience or training in field theory methods will be welcome.

Each of these posts will initially be for 2 years, with a possible extension for a third year. The salary of the successful candidates will depend on their experience (from £22,000 to £30,000 pa).

The starting date for each post is flexible and funding will be available from 1 September, 2006. Although the initial deadline for applications will be 20 June, 2006, the search will continue until all posts are filled. Interested candidates may contact directly either Henning Schomerus (h.schomerus@lancaster.ac.uk) or Vladimir Falko (v.falko@lancaster.ac.uk). For application forms for the vacancies A660, A661, A662 use

http://www.personnel.lancs.ac.uk/CurrentVacancies.aspx

(in your application, please quote the reference number). All candidates are asked to arrange for two reference letters to be sent directly to Dr. Schomerus or Prof. V. Falko, Physics Department, Lancaster University, Lancaster, LA1 4YB, UK (fax: +44 1524 844037).

Professor in Engineering Physics
Helsinki University of Technology (TKK), Finland

Helsinki University of Technology (TKK) announces an opening of a position of a professor in engineering physics. The field of the professorship is specified to be Theoretical physics. The post will be filled either permanently or initially for a period of five years. The post is placed at the Department of Engineering Physics and Mathematics.

Additional information is available from Professor Olavi Nevanlinna email: olavi.nevanlinna@tkk.fi, and administrative manager Dr. Riikka Mäki-Ontto, tel: +358-9-451 3000, email: riikka.maki-ontto@tkk.fi.

The particulars of nomination, which contain information about the position and application procedures, are available from the Registrar's Office of the University, tel: +358-9-451 2030. The particulars of nomination can also be found on the TKK website

http://www.tkk.fi/Yksikot/Hallitus/Virat/index.html.

The application is to be addressed to the Council of Helsinki University of Technology. The closing date for applications is the 27th of June 2006 before 3.45 p.m.

The street address of the Registrar's Office is Otakaari 1, Espoo, and the postal address is Helsinki University of Technology, P.O.Box 1000, FI-02015 TKK, Finland.

Applications can also be delivered by fax or e-mail before the application deadline 27th of June 2006 (TKK, Registrar's Office, fax: +358-9-451 2017, email: kirjaamo@tkk.fi). The details about sending the document electronically can be found in the particulars of nomination.

TEKNILLINEN KORKEAKOULU
TEKNISKA HÖGSKOLAN
HELSINKI UNIVERSITY OF TECHNOLOGY

Postdoctoral Position

”Defect evolution and deformation in metastable alloys”

Department of Materials Science and Engineering, MIT

Applications are invited for one postdoctoral position in the MIT Department of Materials Science and Engineering. This researcher will work with Profs. Sidney Yip, Nicola Marzari, and Krystyn Van Vliet as part of an interdisciplinary, international team that includes strong collaboration with industry partners.

The focus of the project is multiscale computational modeling and simulation of metastable metallic alloys under extreme thermal and mechanical environments. The objective is to identify mechanisms of crystalline defect evolution and consequences toward mechanical deformation.

Funding of this position is for an initial period of 2 years. Demonstrated experience in scientific programming and the application of DFT methods for solid state systems is mandatory; experience with kinetic Monte Carlo and molecular/dislocation dynamics is preferred.

The position is open immediately with a mutually agreed starting date. Requests for further information and applications (CV, two recommenders’ contact information, and one representative publication) should be sent to

Prof. Krystyn J. Van Vliet
Department of Materials Science and Engineering
MIT
E-mail:krystyn@mit.edu

6 Abstracts

Low-temperature magnetization of (Ga,Mn)As semiconductors

T. Jungwirth, J. Mašek
Institute of Physics ASCR, Praha, Czech Republic
K.Y. Wang, K.W. Edmonds, R.P. Campion, L.X. Zhao, C.T. Foxon, B.L. Gallagher
School of Physics and Astronomy, University of Nottingham, UK
M. Sawicki
Institute of Physics, Polish Academy of Sciences, Warszawa, Poland
M. Polini
NEST-INFM and Scuola Normale Superiore, Pisa, Italy
Jairo Sinova, A.H. MacDonald
Department of Physics, Texas A&M University, USA
N.R.S. Farley, T.K. Johal, G. van der Laan
CCLRC Daresbury Laboratory, Warrington WA4 4AD, United Kingdom

Abstract

We report on a comprehensive study of the ferromagnetic moment per Mn in (Ga,Mn)As ferromagnetic semiconductors. Theoretical discussion is based on microscopic calculations and on an effective model of Mn local moments antiferromagnetically coupled to valence band hole spins. The validity of the effective model over the whole range of doping studied is assessed by comparing with microscopic tight-binding/coherent-potential approximation calculations. Using the virtual crystal $\mathrm{k}\cdot\mathrm{p}$ model for hole states, we evaluate zero-temperature mean-field contributions to the magnetization from the hole kinetic energy and exchange energies, and magnetization suppression due to quantum fluctuations of Mn moment orientations around their mean-field ground state values. Experimental low-temperature ferromagnetic moments per Mn are obtained by superconducting quantum interference device and x-ray magnetic circular dichroism in a series of (Ga,Mn)As semiconductors with nominal Mn doping ranging from ∼2% to 8%. Hall measurements in as-grown and annealed samples are used to estimate the number of uncompensated substitutional Mn moments. Based on the comparison between experiment and theory we conclude that all these Mn moments in high-quality (Ga,Mn)As materials have nearly parallel ground state alignment.

Published in Physical Review B **73**, 165205 (2006)
Preprints available from g.vanderlaan@dl.ac.uk

Evidence of a barrier oxidation dependence on the interfacial magnetism in Co/alumina based magnetic tunnel junctions

N. D. Telling, G. van der Laan
Magnetic Spectroscopy Group, Daresbury Laboratory, Warrington WA4 4AD, UK
S. Ladak, R. J. Hicken
University of Exeter, Exeter EX4 4QL, UK
E. Arenholz
Advanced light Source, Berkeley, California 94720

Abstract

Soft x-ray absorption spectroscopy and magnetic circular dichroism at the Co $L_{2,3}$ edge have been applied to explore the near-interfacial magnetism of Co electrodes in Co/alumina based magnetic tunnel junctions. By taking into account the formation of CoO at the ferromagnetic (FM)/barrier interface, the change in the total magnetic moment on metallic Co atoms as a function of barrier oxidation has been determined. The results demonstrate a strong correlation between the Co moments and measured TMR values, and an enhancement in the Co moments for moderate oxidation times.

Accepted for publication in Journal of Applied Physics **99**, 08E505 (2006)
Manuscript available from g.vanderlaan@dl.ac.uk

Direct determination of cation site occupancies in natural ferrite spinels by $L_{2,3}$ X-ray absorption spectroscopy and X-ray magnetic circular dichroism

Carolyn I. Pearce, C. Michael B. Henderson, Richard A.D. Pattrick
School of Earth, Atmospheric and Environmental Sciences
and Williamson Research Centre for Molecular Environmental Science,
The University of Manchester, Manchester M13 9PL, U.K.
Gerrit van der Laan
Synchrotron Radiation Department, CCLRC Daresbury Laboratory,
Daresbury, Warrington WA4 4AD, U.K.
School of Earth, Atmospheric and Environmental Sciences
and Williamson Research Centre for Molecular Environmental Science,
The University of Manchester, Manchester M13 9PL, U.K.
David J. Vaughan
School of Earth, Atmospheric and Environmental Sciences
and Williamson Research Centre for Molecular Environmental Science,
The University of Manchester, Manchester M13 9PL, U.K.

Abstract

Cation distributions in natural ferrite spinels, some containing large amounts of Mg, Ti, Mn, and Zn, have been investigated using the element, site, and symmetry selective spectroscopic techniques of $L_{2,3}$ X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD). By comparing XMCD data with calculated spectra, the site occupancies of the Fe cations have been determined. From the analysis of natural ferrite spinels with formulae very close to that of pure magnetite (Fe_3O_4), a standard XMCD spectrum for natural magnetite is proposed. Magnetites with small numbers of cation vacancies due to oxidation (solid solutions with maghemite, γ-Fe_2O_3) show that all the vacancies occur in octahedral sites. Ti $L_{2,3}$ XAS of oxidized Ti-bearing magnetites (hereafter referred to titanomagnetites) shows that Ti is tetravalent occurring on the octahedral site with $10Dq \sim 2$eV; Fe $L_{2,3}$ XMCD spectra indicate that the vacancies occur in both tetrahedral and octahedral sites. Mn $L_{2,3}$ XAS of the Mn-rich ferrite spinels shows that Mn is predominantly ordered onto the tetrahedral site with an $Mn^{2+} : Mn^{3+}$ ratio of $0.85 : 0.15$. Mn- and Zn-rich ferrite spinels have an excess of cations over 3.0 per 4-oxygen formula unit. The sign of the XMCD for Mn corresponds to a parallel alignment of the Mn moments with the Fe^{3+} moments in the tetrahedral sublattice. This work demonstrates clearly that combined XAS and XMCD provides direct information on the distribution of multivalent cations in chemically complex magnetic spinels.

Published in American Mineralogist **91**, 880–893 (2006)
Manuscript available from g.vanderlaan@dl.ac.uk

Efficient solution of Poisson's equation with free boundary conditions

Luigi Genovese, Thierry Deutsch
Département de recherche fondamentale sur la matière condensée,
SP2M/L_Sim, CEA-Grenoble, 38054 Grenoble cedex 9, France
Alexey Neelov, Stefan Goedecker
Institute of Physics, University of Basel,
Klingelbergstrasse 82, CH-4056 Basel, Switzerland
Gregory Beylkin
Department of Applied Mathematics, University of Colorado at Boulder,
Boulder, Colorado 80309-0526

Abstract

Interpolating scaling functions give a faithful representation of a localized charge distribution by its values on a grid. For such charge distributions, using a Fast Fourier method, we obtain highly accurate electrostatic potentials for free boundary conditions at the cost of O(N logN) operations, where N is the number of grid points. Thus, with our approach, free boundary conditions are treated as efficiently as the periodic conditions via plane wave methods.

(submitted to: Journal of Chemical Physics)
Latex-file available from http://arxiv.org/abs/cond-mat/0605371

Linear scaling calculation of maximally-localized Wannier functions with atomic basis set

H. J. Xiang, Zhenyu Li, W. Z. Liang, Jinlong Yang, J. G. Hou, and Qingshi Zhu
Hefei National Laboratory for Physical Sciences at Microscale,
University of Science and Technology of China,
Hefei, Anhui 230026, People's Republic of China

Abstract

We have developed a linear scaling (O(N)) algorithm for calculating maximally-localized Wannier functions (MLWFs) using atomic orbital basis. An O(N) ground state calculation is carried out to get the density matrix (DM). Through a projection of the DM onto atomic orbitals and a subsequent O(N) orthogonalization, we obtain initial orthogonal localized orbitals. These orbitals can be maximally localized in linear scaling by simple Jacobi sweeps. Our O(N) method is validated by applying it to water molecule and wurtzite ZnO. The linear scaling behavior of the new method is demonstrated by computing the MLWFs of boron nitride nanotubes.

(To be published in Journal of Chemical Physics, cond-mat/0605047)
Contact person: xhongjun@mail.ustc.edu.cn

Exchange interactions and Curie temperatures in $Ni_{2-x}MnSb$ alloys

Ján Rusz[1,2], Lars Bergqvist[3], Josef Kudrnovský[2], Ilja Turek[1]
[1] *Dept. of Electronic Structures, Charles University, Prague*
[2] *Institute of Physics, ASCR, Prague*
[3] *Dept. of Physics, Uppsala University, Sweden*

Abstract

We present the first-principles study of physical properties of the disordered $Ni_{2-x}MnSb$ alloys which form a continuous series connecting two typical members of Heusler alloy family, namely the halfmetallic semi-Heusler alloy NiMnSb ($x = 1$) and related metallic Heusler alloy Ni_2MnSb ($x = 0$). Magnetic moments, exchange interactions, magnon-spectra, and Curie temperatures at ambient and elevated pressures are determined and compared with available experimental data. The spin-spin correlation functions at the critical temperature are also calculated. The pair exchange interactions and corresponding classical Heisenberg Hamiltonian are derived from self-consistent electronic structure calculations using a magnetic force theorem. Heusler alloys NiMnSb and Ni_2MnSb exhibit strikingly different asymptotic behavior of exchange interactions with the distance between magnetic atoms. The Curie temperatures are estimated using multi-sublattice versions of the mean-field approximation, random-phase approximation, and Monte Carlo simulations. The robustness of results with respect to the effect of correlations beyond the local density approximation, the selected reference state used for mapping to the Heisenberg Hamiltonian and the applied mapping procedure are also discussed.

(Physical Review B, in print)
Contact person: Ján Rusz, rusz@mag.mff.cuni.cz

Exchange interactions and crystal-field effects in HoX (X = Ag, Cd, Cu, Mg, Rh, Zn) intermetallic compounds

Ján Rusz[1,2], Ilja Turek[1,3], Martin Diviš[1]
[1] *Dept. of Electronic Structures, Charles University, Prague*
[2] *Institute of Physics, ASCR, Prague*
[3] *Institute of Physics of Materials, ASCR, Brno*

Abstract

We present an ab initio treatment of the exchange interactions and crystal-field effects in HoX (X = Ag, Cd, Cu, Mg, Rh, Zn) intermetallic compounds with the CsCl crystal structure. The exchange interactions are determined using the magnetic-force theorem starting from both a ferromagnetically ordered state (zero temperature) and a disordered-local-moments (effectively high temperature) state up to an interatomic distance of $10a$, where a is the lattice parameter. The exchange interactions are used for construction of the Heisenberg Hamiltonian, from which we determine the magnetic-transition temperatures using the mean-field approximation and the Green's-function based random-phase approximation. The crystal-field parameters are derived from an ab initio electronic structure of the non-magnetic state. A combined Hamiltonian is treated within the mean-field approximation to study the effect of the crystal-field interaction on the critical temperatures and the magnetization.

(Physica B: Cond. Matt. 381 (2006), 265-270)

Contact person: Ján Rusz, rusz@mag.mff.cuni.cz

Surface reconstructions and atomic ordering in $In_xGa_{1-x}As(001)$ films: a first-principles study

Aparna Chakrabarti
Raja Ramanna Centre for Advanced Technology, Indore 452013, India

Peter Kratzer and Matthias Scheffler
Fritz-Haber-Institut der MPG, D-14195 Berlin-Dahlem, Germany

Abstract

Density-functional theory calculations are carried out for various surface reconstructions of atomically ordered thin films of $In_xGa_{1-x}As$ on the (001)-oriented InP substrate for compositions close to x=1/2. In addition to the known $(n \times 3)$ and (2×4) reconstructions, a gallium-rich $\zeta(4 \times 2)$ reconstruction, so far only observed for binary arsenides, is predicted for growth conditions poor in arsenic and indium. Moreover, the possibility of a $c(4 \times 4)$ reconstruction, either purely terminated by As–As dimers or mixed with heterodimers, as well as the possible occurrence of heterodimers in other reconstructions have been investigated. From our calculated film formation energies, these reconstructions is expected to play a minor role for (In,Ga)As films under thermodynamic equilibrium conditions. For the surface-induced atomic ordering in the (In,Ga)As films, our calculations are in line with known trends for (In,Ga)P alloys: $CuPt_B$-type ordering in the cation lattice is energetically preferable for most growth conditions apart from very anion-rich conditions, where triple-period ordering or $CuPt_A$-type ordering in conjunction with the $(n \times 3)$ or $c(4 \times 4)$ surface reconstruction, respectively, becomes preferable. In general, the energetic preference for near-surface ordering in the (In,Ga)As system is found to be somewhat weaker than in the (In,Ga)P system.

(submitted to: Phys. Rev. B)

Contact person: Peter Kratzer (Peter.Kratzer@uni-due.de)

Diffusion Pathways of Hydrogen across the Steps of a vicinal Si(001) Surface

M. Lawrenz, C. H. Schwalb, M. Dürr, and U. Höfer
Fachbereich Physik und Zentrum für Materialwissenschaften,
Philipps-Universität, D-35032 Marburg, Germany

P. Kratzer
Fritz-Haber-Institut der MPG, D-14195 Berlin-Dahlem, Germany

Abstract

Hydrogen diffusion across D_B steps on Si(001)-surfaces was investigated by means of variable-temperature scanning tunneling microscopy and first-principles calculations. Experimentally, the hopping rate for diffusion from the step sites to the Si-dimers of the upper terrace was found to be more than one order of magnitude higher than for diffusion to the lower terrace. This clear preference, opposite to the trend for the respective binding energies, is explained by first-principles calculations that identify a meta-stable intermediate to be responsible for the unexpected lowering of the energy barrier for upward diffusion.

(submitted to: Phys. Rev. Lett.)
Contact person: Peter Kratzer (Peter.Kratzer@uni-due.de)

Shape Transition during Epitaxial Growth of InAs Quantum Dots on GaAs(001): Theory and Experiment

P. Kratzer
Fritz-Haber-Institut der MPG, D-14195 Berlin-Dahlem, Germany
Q. K. K. Liu
Hahn-Meitner-Institut, D-14109 Berlin, Germany
P. Acosta-Diaz, C. Manzano, G. Costantini, R. Songmuang,
A. Rastelli, O. G. Schmidt, and K. Kern
Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart

Abstract

For heteroepitaxial growth of InAs islands on GaAs(001), a transition of shapes is observed experimentally by scanning-tunneling microscopy and analyzed theoretically in terms of the thermodynamic stability of the islands. The experiments show the co-existence of small islands bound predominantly by shallow facets of the {137} family and large islands that show a variety of steeper facets, among them the {101}, {111}, and $\{\bar{1}\bar{1}\bar{1}\}$ orientations. The calculations of island stability employ a hybrid approach where the elastic strain relief in the islands is calculated by continuum elasticity theory, while surface energies and surface stresses are taken from density-functional theory calculations that take into account the atomic structure of the various side facets, as well as of the InAs wetting layer on GaAs(001). With the help of the theoretical analysis, we interpret the observed co-existence of shapes in terms of a structural phase transition accompanied by a discontinuous change of the chemical potential in the islands. Consequences of this finding are discussed in analogy with a similar behavior of GeSi islands on silicon observed previously.

(submitted to: Phys. Rev. B)
Contact person: Peter Kratzer (Peter.Kratzer@uni-due.de)

Quasiparticle Calculations for Point Defects at Semiconductor Surfaces

Arno Schindlmayr[1,2] and Matthias Scheffler[2]
[1]*Institut für Festkörperforschung, Forschungszentrum Jülich,*
52425 Jülich, Germany
[2]*Fritz-Haber-Institut der Max-Planck-Gesellschaft,*
Faradayweg 4–6, 14195 Berlin-Dahlem, Germany

Abstract

We present a quantitative parameter-free method for calculating defect states and charge-transition levels of point defects in semiconductors. It combines the strength of density-functional theory for ground-state total energies with quasiparticle corrections to the excitation spectrum obtained from many-body perturbation theory. The latter is implemented within the G_0W_0 approximation, in which the electronic self-energy is constructed non-self-consistently from the Green function of the underlying Kohn–Sham system. The method is general and applicable to arbitrary bulk or surface defects. As an example we consider anion vacancies at the (110) surfaces of III–V semiconductors. Relative to the Kohn–Sham eigenvalues in the local-density approximation, the quasiparticle corrections open the fundamental band gap and raise the position of defect states inside the gap. As a consequence, the charge-transition levels are also pushed to higher energies, leading to close agreement with the available experimental data.

(submitted to: *Theory of Defects in Semiconductors*, edited by D. A. Drabold and S. K. Estreicher, Springer Series "Topics in Applied Physics")
Contact person: Arno Schindlmayr (A.Schindlmayr@fz-juelich.de)

Density Functional Theory Simulations of Water-Metal Interfaces: Waltzing Waters, a Novel 2D Ice Phase, and More

Angelos Michaelides
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14195 Berlin, Germany

Abstract

There are few molecules, if any, more important than water. Yet remarkably little is known about how it interacts with solid surfaces, particularly at the all important atomic-level. This is true despite widespread general interest and compelling environmental and economic incentives. Here, I will discuss detailed density-functional theory studies aimed at putting our understanding of water-solid interfaces, specifically water-metal interfaces, on a much firmer footing. Some of the key questions I will attempt to answer are: Where do isolated water monomers adsorb on flat metal surfaces? How do water monomers diffuse across metal surfaces? How do water dimers adsorb and diffuse across metal surfaces? What factors control the structure and stability of water bilayers on metal surfaces?

(submitted to Applied Physics A)
Contact person: Angelos Michaelides (michaeli@fhi-berlin.mpg.de)

Diabatic Potential-Energy Surfaces by Constrained Density-Functional Theory

Jörg Behler[1], Bernard Delley[2], Karsten Reuter[1], Matthias Scheffler[1]
[1] *Fritz-Haber-Institut der Max-Planck-Gesellschaft,*
Faradayweg 4-6, D-14195 Berlin, Germany
[2] *Paul-Scherrer-Institut, HGA/123, CH-5232 Villigen PSI, Switzerland*

Abstract

Nonadiabatic effects play an important role in many chemical processes. In order to study the underlying diabatic potential-energy surfaces (PESs), we present a locally-constrained density-functional theory approach, which enables us to confine electrons to sub-spaces of the Hilbert space, e.g. to selected atoms or groups of atoms. This allows to calculate diabatic PESs for defined charge and spin states of the chosen subsystems. The capability of the method is demonstrated by calculating diabatic PESs for the scattering of a sodium and a chlorine atom, for the interaction of a chlorine molecule with a small metal cluster, and for the dissociation of an oxygen molecule at the Al(111) surface.

(submitted to: Physical Review B)

Contact person: Jörg Behler (behler@fhi-berlin.mpg.de)

Electronic Structure of Spinel Ferrites

Z. Szotek[1], W.M. Temmerman[1], D. Ködderitzsch[2], A. Svane[3], L. Petit[4],
and H. Winter[5]
[1] *Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, Cheshire, U.K.*
[2] *Physikalische Chemie, Ludwig-Maximilian University, Munich, Germany*
[3] *Department of Physics and Astronomy, University of Aarhus,*
DK-8000 Aarhus C, Denmark
[4] *Computer Science and Mathematics Division,*
and Center for Computational Sciences, Oak Ridge National Laboratory,
Oak Ridge, TN 37831, USA
[5] *IFP, Forschungszentrum Karlsruhe GmbH,*
Postfach 3640, D-76021 Karlsruhe, Germany

Abstract

We apply the self-interaction corrected local spin density approximation to study the electronic structure and magnetic properties of the spinel ferrites $MnFe_2O_4$, Fe_3O_4, $CoFe_2O_4$, and $NiFe_2O_4$. We concentrate on establishing the nominal valence of the transition metal elements and the ground state structure, based on the study of various valence scenarios for both the inverse and normal spinel structures for all the systems. For both structures we find all the studied compounds to be insulating, but with smaller gaps in the normal spinel scenario. On the contrary, the calculated spin magnetic moments and the exchange splitting of the conduction bands are seen to increase dramatically when moving from the inverse spinel structure to the normal spinel kind. We find substantial orbital moments for $NiFe_2O_4$ and $CoFe_2O_4$.

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Contact person: Z.Szotek@dl.ac.uk

Lattice Dynamics of MgO at High Pressure: Theory and Experiment

Subrata Ghose, Michael Krisch, Artem R. Oganov, Alexandre Beraud, Alexey Bosak,
Revansidha Gulve, Raghunandan Seelaboyina, Hexiong Yang, and Surendra K. Saxena
ETH Zürich, Switzerland

Abstract

The longitudinal acoustic and optical phonon branches along the Gamma-X direction of MgO at 35 GPa have been determined by inelastic x-ray scattering using synchrotron radiation and a diamond-anvil cell. The experimentally observed phonon branches are in remarkable agreement with ab initio lattice dynamics results. The derived thermodynamic properties, such as the specific heat CV and the entropy S are in very good accord with values obtained from a thermodynamically assessed dataset involving measured data on molar volume, heat capacity at constant pressure, bulk modulus and thermal expansion.

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Contact person and reprints contact: Artem R. Oganov (a.oganov@mat.ethz.ch)

Ab initio molecular dynamics study of $CaSiO_3$ perovskite at P-T conditions of Earth's lower mantle

Donat J. Adams and Artem R. Oganov
ETH Zürich, Switzerland

Abstract

First-principles molecular dynamics calculations were performed in order to investigate the structure and properties of what is thought to be the third most abundant phase in the Earth's lower mantle, $CaSiO_3$ perovskite. The commonly assumed cubic structure was found to be stable at high temperatures T $\sim$ 1000-2000 K, and unstable at low temperatures at all pressures. For this structure we investigate the thermal equation of state and the Grüneisen parameter. We predict that the ground state of $CaSiO_3$ perovskite is tetragonal (space group I4/mcm). At room temperature an orthorhombic structure (space group Imma) is possible, which explains puzzling experimental X-ray powder diffraction patterns. We consider the structure relation between the Imma and the I4/mcm structures and show that the Imma structure can be obtained by a counterintuitive symmetry-lowering transition on increasing temperature.

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Contact person: Artem R. Oganov (a.oganov@mat.ethz.ch)

Effect of hydrostatic pressure on the crystal structure of sodium oxalate: X-ray diffraction study and ab initio simulations

Elena V. Boldyreva, Hans Ahsbahs, Vladimir V. Chernyshev,
Svetlana N. Ivashevskaya, and Artem R. Oganov
ETH Zürich, Switzerland

Abstract

Effect of hydrostatic pressures up to 8 GPa on the crystals of $Na_2C_2O_4$ (sp. gr. P21/c) was studied in situ in the diamond anvil cells a)in neon,b)in methanol-ethanol mixture by high-resolution X-ray powder diffraction (synchrotron radiation). Below 3.3-3.8 GPa, anisotropic structural distortion was observed, which was similar to, but not identical with that on cooling. At 3.8 GPa, a reversible isosymmetric first-order phase transition without hysteresis occurred.The orientation of the oxalate anions changed at the transition point by a jump, and so did the coordination of the sodium cations by oxygen atoms. Ab initio simulations based on the generalized gradient approximation of density functional theory have reproduced the main features of the structural changes in the crystals of sodium oxalate with increasing pressure. The theoretical pressure for the isosymmetric phase transition is 3.65 GPa,close to the experimental value; in agreement with experiment the transition was predicted to be reversible. Ab initio calculations gave a pronounced hysteresis for this transition, and have also predicted a further isosymmetric phase transition at 10.9 GPa, also with a hysteresis. The role of temperature in the pressure-induced phase transitions in sodium oxalate is discussed.

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Contact person and reprints contact: Artem R. Oganov (a.oganov@mat.ethz.ch)

Origin of the negative volume magnetostriction of the intermetallic compound $GdAl_2$

I. Turek, J. Rusz and M. Diviš
Faculty of Mathematics and Physics, Department of Electronic Structures,
Charles University in Prague, Czech Republic

Abstract

Spontaneous volume magnetostriction of the intermetallic compound $GdAl_2$ with a cubic C15 Laves structure is studied from first principles using the local spin-density approximation combined optionally with an open-core treatment of the atomic-like Gd-$4f$ orbitals. Local magnetic moments and equilibrium lattice parameters are evaluated for two spin structures, namely for the ferromagnetic ground state and for a state with randomly oriented Gd moments. The resulting spontaneous volume magnetostriction compares well with experimentally observed values; its negative sign however cannot be ascribed to a variation of the size of the local Gd moment but has its origin in the volume dependence of exchange interactions between the Gd moments. The Curie temperature and its pressure dependence are derived from the calculated pair exchange interactions as well; their values are found in reasonable agreement with experiment supporting thus the above explanation of the anomalous magnetoelastic behavior of the $GdAl_2$ compound.

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Contact person: Ilja Turek (turek@ipm.cz).

The Perdew-Burke-Ernzerhof exchange-correlation functional applied to the G2-1 test set using a plane-wave basis set

Joachim Paier, Robin Hirschl, Martijn Marsman, and Georg Kresse
Institut für Materialphysik and Center for Computational Materials Science,
Universität Wien,Sensengasse 8/12, A-1090 Wien, Austria

Abstract

Present local and semi-local functionals show significant errors for instance in the energetics of small molecules and in the description of band gaps. One possible solution to these problems is the introduction of exact exchange and hybrid functionals. A plane-wave based algorithm was implemented in VASP (*Vienna Ab-initio Simulation Package*) to allow for the calculation of exact exchange. To systematically assess the precision of the present implementation, calculations for the 55 molecules of the G2-1 quantum chemical test set were performed applying the PBE and PBE0 functionals. Excellent agreement for both atomization energies and geometries compared to the results obtained by GAUSSIAN 03 calculations using large basis sets (aug-cc-pVQZ for the geometry optimization, aug-cc-pV5Z for the energy calculations) was found. The mean absolute error (MAE) for atomization energies between VASP and the experiment is 8.6 kcal/mol and 3.7 kcal/mol, as calculated with the PBE functional and PBE0 respectively. The mean deviations between VASP and GAUSSIAN are 0.46 kcal/mol and 0.49 kcal/mol for the PBE and PBE0 functional, respectively.

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Contact person: joachim.paier@univie.ac.at

Screened hybrid density functionals applied to solids

J. Paier, M. Marsman, K. Hummer, and G. Kresse
Institut für Materialphysik and Center for Computational Materials Science,
Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria
I. C. Gerber and J. G. Ángyán
Laboratoire de Cristallographie et de Modélisation des Matériaux Minéraux et Biologiques,
UMR 7036, Université Henri Poincaré, B.P. 239, F-54506 Vandœuvre-lès-Nancy, France

Abstract

Hybrid Fock exchange/density functional theory functionals have shown to be very successful in describing a wide range of molecular properties. For periodic systems, however, the long-range nature of the Fock exchange interaction and the resultant large computational requirements present a major drawback. This is especially true for metallic systems, which require a dense Brillouin zone sampling. Recently, a new hybrid functional [HSE03, J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. **118**, 8207 (2003)] that addresses this problem within the context of methods that evaluate the Fock exchange in real space was introduced. We discuss the advantages the HSE03 functional brings to methods that rely on a reciprocal space description of the Fock exchange interaction, e.g., all methods that use plane wave basis sets. Furthermore, we present a detailed comparison of the performance of the HSE03 and PBE0 functionals for a set of archetypical solid state systems, by calculating lattice parameters, bulk moduli, heats of formation and band gaps. The results indicate that the hybrid functionals, indeed often improve the description of these properties, but in several cases the results are not yet on par with standard gradient corrected functionals. This concerns in particular metallic systems for which the bandwidth and exchange splitting are seriously overestimated.

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Contact person: joachim.paier@univie.ac.at

Implementation of dynamical mean-field theory using Wannier functions: a flexible route to electronic structure calculations of strongly correlated materials

F. Lechermann
Centre de Physique Théorique, École Polytechnique,
91128 Palaiseau Cedex, France
LPT-ENS, 24 Rue Lhomond, 75231 Paris Cedex 05, France
A. Georges
Centre de Physique Théorique, École Polytechnique,
91128 Palaiseau Cedex, France
A. Poteryaev
Centre de Physique Théorique, École Polytechnique,
91128 Palaiseau Cedex, France
S. Biermann
Centre de Physique Théorique, École Polytechnique,
91128 Palaiseau Cedex, France
M. Posternak
Institute of Theoretical Physics, Ecole Polytechnique Fédérale,
de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
A. Yamasaki
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1,
D-70569, Stuttgart, Germany
O.K. Andersen
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1,
D-70569, Stuttgart, Germany

Abstract

A versatile method for combining density functional theory (DFT) in the local density approximation (LDA) with dynamical mean-field theory (DMFT) is presented. Starting from a general basis-independent formulation, we use Wannier functions as an interface between the two theories. These functions are used for the physical purpose of identifying the correlated orbitals in a specific material, and also for the more technical purpose of interfacing DMFT with different kinds of band-structure methods (with three different techniques being used in the present work). We explore and compare two distinct Wannier schemes, namely the maximally-localized-Wannier-function (MLWF) and the N-th order muffin-tin-orbital (NMTO) methods. Two correlated materials with different degrees of structural and electronic complexity, $SrVO_3$ and $BaVS_3$, are investigated as case studies. $SrVO_3$ belongs to the canonical class of correlated transition-metal oxides, and is chosen here as a test case in view of its simple structure and physical properties. In contrast, the sulfide $BaVS_3$ is known for its rich and complex physics, associated with strong correlation effects and low-dimensional characteristics. New insights into the physics associated with the metal-insulator transition of this compound are provided, particularly regarding correlation-induced modifications of its Fermi surface. Additionally, the necessary formalism for implementing self-consistency over the electronic charge density in a Wannier basis is discussed.

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Contact person: Frank.Lechermann@cpht.polytechnique.fr

Hyperfine Interactions at Lanthanide Impurities in Iron

D. Torumba, S. Cottenier, V. Vanhoof, M. Rots
Instituut voor Kern- en Stralingsfysica and INPAC
Celestijnenlaan 200D, BE-3001 Leuven, Belgium

Abstract

The magnetic hyperfine field and electric-field gradient at isolated lanthanide impurities in an Fe host lattice are calculated from first principles, allowing a qualitative and quantitative understanding of an experimental data set collected over the past 40 years. It is demonstrated that the common Local Density Approximation leads to quantitatively and qualitatively wrong results, while the LDA+U method performs much better. In order to avoid pitfalls inherent to the LDA+U method, a combination of free ion calculations and 'constrained density matrix' calculations is proposed and tested. Quantitative results for the exchange field and crystal field parameters are obtained (B_{exc}=+420 T, $B_0^4 = -1000$ cm^{-1}, $B_0^6 = -800$ cm^{-1}), showing in particular how crystal field effects influence the hyperfine fields for the lightest and the heaviest lanthanides. The hyperfine fields are shown to be dominated by the 4f orbital contribution, with small corrections due to the spin dipolar and Fermi contact fields. The latter is found to be constant for all lanthanides, a feature that is understood by a modified version of the well-known core polarization mechanism for 3d hyperfine fields. Spin dipolar fields and electric-field gradients have apart from a 4f contribution a surprisingly strong contribution due to the completely filled lanthanide 5p orbitals – the mechanism behind this is explained. The lanthanide 4f spin moment is found to couple antiparallel to the magnetization of the Fe lattice, in agreement with the model of Campbell and Brooks. There is strong evidence for a delocalization-localization transition that is shifted from Ce to at least Pr and maybe further up to Sm. This shift is interpreted in terms of the effective pressure felt by lanthanides in Fe. Implications for resolving ambiguities in the determination of delocalization in pure lanthanide metals under pressure are discussed. For the localized lanthanides, Yb is shown to be divalent in this host lattice, while all others are trivalent (including Eu). The temperature dependence of the hyperfine fields is discussed as well.

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pdf-file available from Stefaan.Cotttenier@fys.kuleuven.be

Ab-initio study of the surface of a decagonal AlCoNi quasicrystal

M. Krajčí[a,b], J. Hafner[a], and M. Mihalkovič[b]
[a] *Institut für Materialphysik*
and Center for Computational Materials Science, Universität Wien,
Sensengasse 8/12, A-1090 Wien, Austria
[b] *Institute of Physics, Slovak Academy of Sciences,*
Dúbravská cesta 9, SK-84511 Bratislava, Slovak Republic

Abstract

The structure, stability and electronic properties of the tenfold-fold surface of the decagonal AlCoNi quasicrystal have been investigated using ab-initio density-functional methods. The structural model of the surface has been derived from the recently resolved structure of the W-(AlCoNi) approximant phase. The bulk quasicrystal can be cleaved at the flat A plane or at the puckered B plane. We investigate the stability and the electronic properties of the surface for both possible terminations. The simulated STM images of the A and B surfaces show that despite their significantly different atomic structure and chemical composition of both surfaces exhibit quite similar STM images. The electronic structure of the approximant phase is characterized by a pseudogap at the Fermi level. The pseudogap at the surface is partially covered and the positions of d-bands of both transition metals undergo a substantial shift towards lower binding energies.

(Phys. Rev. B **73**, 134203 (2006))
Contact person: fyzikraj@savba.sk

Ab-initio study of quasiperiodic Bi monolayers on a tenfold d-Al-Co-Ni surface

M. Krajčí[a,b], J. Hafner[a], and M. Jahnátek[a,b]
[a] *Institut für Materialphysik*
and Center for Computational Materials Science, Universität Wien,
Sensengasse 8/12, A-1090 Wien, Austria
[b] *Institute of Physics, Slovak Academy of Sciences,*
Dúbravská cesta 9, SK-84511 Bratislava, Slovak Republic

Abstract

We present an ab-initio study of the formation of quasiperiodic Bi monolayers on the tenfold surface of a decagonal Al-Co-Ni quasicrystal. The structural model of the surface has been derived from the recently resolved structure of the W-(AlCoNi) approximant phase. As the bulk W-phase can be cleaved at the flat A plane or the puckered B plane we investigate the formation and stability of the monolayers on both surfaces. The structural model of a Bi monolayer adsorbed on the tenfold surface has been constructed on the basis of a mapping of the potential-energy landscape of an isolated Bi adatom on the substrate. We found stable quasiperiodic monolayers on both surfaces. The structure of the monolayer on the B-surface is less dense and more regular than that on the A-surface. The surface coverages are within the experimentally determined range $\simeq 0.08 \pm 0.02$ atoms/Å^2.

(Phys. Rev. B, in print)

Contact person: fyzikraj@savba.sk

High-field magnetic susceptibility of $Fe_{1-x}Co_x$ alloys

S. Mankovsky and H. Ebert
Department Chemie und Biochemie/Physikalische Chemie,
Universität München,
Butenandtstr. 5-13, D-81377 München, Germany

Abstract

A fully relativistic theoretical description of the magnetic high-field susceptibility of disordered alloys is presented. This approach not only accounts for the Pauli spin and Van Vleck orbital susceptibilities considered so far in this context, but also for the spin-orbit induced contributions as well as the Landau susceptibility. Applications to $Fe_{1-x}Co_x$ alloys led to a very good agreement with experiment for the Fe-rich side of the system. This also applies for the middle concentration regime if a partial ordering of the samples is accounted for in the calculations. In contrast to prior investigations on the ferromagnets Fe, Co, and Ni, that considered only the Pauli spin susceptibility, it could be shown that the orbital Van Vleck and Landau contributions to the susceptibility dominate.

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Contact person: S.Mankovsky
e-mail address: Sergiy.Mankovskyy@cup.uni-muenchen.de

Magnetic properties of free Fe clusters at finite temperatures from first principles

S. Polesya[1], O. Šipr[2], S. Bornemann[1], J. Minár[1]
H. Ebert[1]
[1] *Universität München, Department Chemie,*
Butenandtstr. 5-13, D-81377 München, Germany
[2] *Institute of Physics, Academy of Sciences of the Czech Republic,*
Cukrovarnická 10, CZ-162 53 Prague, Czech Republic

Abstract

An *ab initio* theoretical investigation on the finite-temperature magnetism of free metallic clusters is presented. The exchange coupling between local magnetic moments in Fe clusters of 9–89 atoms was calculated within the mulUniversität Münchentiple-scattering formalism. From the results an effective classical Heisenberg Hamiltonian was constructed, and the magnetization as a function of temperature was obtained via Monte Carlo simulations. It is found that the effective critical temperature is not a monotonous function of the cluster size. We demonstrate that for a proper description of finite-temperature magnetism of free clusters, the site-dependence of the exchange coupling must be taken into account.

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Contact person: Svitlana.Polesya@cup.uni-muenchen.de

An efficient implementation of the Korringa-Kohn-Rostoker non-local coherent-potential approximation with a fully relativistic application to the ferromagnetic alloy system FePt

D. Ködderitzsch[1], H. Ebert[1], D. A. Rowlands[2], A. Ernst[3]
1 Ludwig-Maximilians-Universität München,
Department Chemie und Biochemie, Physikalische Chemie, München
2 H. H. Wills Physics Laboratory, University of Bristol, UK
3 Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Abstract

The recently devised extension of the Korringa-Kohn-Rostoker Coherent Potential Approximation (KKR-CPA) to the non-local KKR-NLCPA provides a sound basis to include systematically local environmental effects in an *ab initio* description of disordered systems. Here we show how a reformulation of the KKR-NLCPA condition lends hand to a stabilisation of convergence in the self-consistent determination of the effective medium. Further we show how one can greatly reduce the computational effort in the coarse graining procedure by making use of symmetry. Our formulation includes the standard non-relativistic as well as the extension to the fully relativistic case of the KKR-NLCPA. We apply our approach to a particular system, namely FePt, and study the influence of local environmental effects on its electronic and magnetic properties.

(Submitted to Phys. Rev. B)

Contact person: D. Ködderitzsch (diemo.koedderitzsch@cup.uni-muenchen.de)

Present Address: Ludwig-Maximilians-Universität München
Department Chemie und Biochemie, Physikalische Chemie
Butenandtstraße 11
D-81377 München

Density functional theory for disordered alloys with short-range order: systematic inclusion of charge-correlation effects

D. A. Rowlands[1], A. Ernst[2], B. L. Gyorffy[1], and J. B.Staunton[3]
1. H.H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, U.K.
2. Max Planck Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany
ewline *3. Dept. of Physics, University of Warwick, Coventry CV4 7AL, U.K.*

Abstract

For many years, density functional-based calculations for the total energies of substitutionally-disordered alloys have been based upon the Korringa-Kohn-Rostoker coherent-potential approximation (KKR-CPA). However, as a result of the single-site nature of the KKR-CPA, such calculations do not take into account important local environmental effects such as charge correlations (the Madelung energy) and chemical short-range order (SRO). Here the above approach is generalized by combining the recently developed Korringa-Kohn-Rostoker nonlocal coherent-potential approximation (KKR-NLCPA) with density functional theory, showing how these effects may be systematically taken into account. As a first application of the theory, total energy calculations for the *bcc* $Cu_{50}Zn_{50}$ solid solution are presented, showing how the total energy varies as a function of SRO. The fcc $Cu_{60}Pd_{40}$ and $Cu_{77}Ni_{23}$ systems are also investigated.

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Contact person: d.a.rowlands@bristol.ac.uk

Investigation of the nonlocal coherent-potential approximation

D. A. Rowlands
H.H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, U.K.

Abstract

Recently the nonlocal coherent-potential approximation (NLCPA) has been introduced by Jarrell and Krishnamurthy for describing the electronic structure of substitutionally-disordered systems. The NLCPA provides systematic corrections to the widely used coherent-potential approximation (CPA) whilst preserving the full symmetry of the underlying lattice. Here an analytical and systematic numerical study of the NLCPA is presented for a one-dimensional tight-binding model Hamiltonian, and comparisons with the embedded cluster method (ECM) and molecular coherent potential approximation (MCPA) are made.

(Journal Reference: J. Phys.:Condens. Matter 18, 3179-3195 (2006))
Contact person: d.a.rowlands@bristol.ac.uk

First-principles investigation of Co wires at Pt(111) step-edges

S. Baud
Laboratoire de physique moléculaire, UMR
CNRS 6624, Université de Franche-Comté, F-25030
Besançon Cedex, France
G. Bihlmayer and S. Blügel
Institut für Festkörperforschung,
Forschungszentrum Jülich, D-52425 Jülich, Germany
Ch. Ramseyer
Laboratoire de physique moléculaire, UMR
CNRS 6624, Université de Franche-Comté, F-25030
Besançon Cedex, France

Abstract

We report on *ab initio* calculations of Pt(111) B-type step-edges decorated with Co chains of different thickness. As found experimentally, these Co n-wires show for $n = 1$ (monowire) a large magnetic anisotropy that decreases for larger n in a non-monotonous way. Also the easy axis shows a oscillatory behavior with increasing n that can be traced back to competing effects arising from different strands of the thicker wires.

(Accepted at Surface Science)

Contact person: G.Bihlmayer@fz-juelich.de

The Rashba-effect at metallic surfaces

G. Bihlmayer
Institut für Festkörperforschung,
Forschungszentrum Jülich, D-52425 Jülich, Germany
Yu. M. Koroteev
Institute of Strength Physics and Materials Science,
Russian Academy of Sciences, 634021, Tomsk, Russia
P. M. Echenique and E. V. Chulkov
Departamento de Fisica de Materiales and Centro Mixto CSIC-UPV/EHU,
Facultad de Ciencias Quimicas, UPV/EHU, Apdo.1072, 20080
San Sebastian/Donostia, Basque Country, Spain
S. Blügel
Institut für Festkörperforschung,
Forschungszentrum Jülich, D-52425 Jülich, Germany

Abstract

Surface states, that show a **k**-dependent splitting resulting from spin-orbit coupling, show wide similarities to a two-dimensional electron gas in semiconductor heterostructures, where the Rashba effect lifts the spin-degeneracy of the bands and allows spin-manipulation by an electric field. We discuss the conditions for such a Rashba-effect at metallic surfaces by comparing *ab initio* calculations for Au(111), Ag(111), and Lu(0001) and investigate the influence of electric and magnetic (exchange) fields on these surface states.

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Contact person: G.Bihlmayer@fz-juelich.de

Charge localization or itineracy at $LaAlO_3/SrTiO_3$ interfaces: hole polarons, oxygen vacancies, and mobile electrons

R. Pentcheva
Dept. of Earth and Environmental Sciences, University of Munich,
Theresienstr. 41, 80333 Munich, Germany
and Department of Geology, University of California, Davis, CA 95616
W.E. Pickett
Department of Physics, University of California, Davis, CA 95616

Abstract

While correlated electron behavior is to be expected at oxide interfaces (IFs) involving Mott insulators, we show how strong correlations in the oxygen $2p$-states may be necessary to account for observed insulating behavior at charged (001)-IFs between the band insulators $LaAlO_3$ and $SrTiO_3$. Using correlated band theory applied to the O $2p$-states, an insulating p-type IF is obtained only when a disproportionated, charge-, orbital-, and spin-ordered O P_π magnetic hole is formed, centered between Al^{3+}-ions in the AlO_2-layer at the IF. As an alternative explanation, charge compensation by oxygen vacancies that accommodate the holes as charge-conjugate F-centers is modeled. For the n-type IF, a charge disproportionated Ti^{4+}+Ti^{3+}-layer is obtained with ferromagnetic alignment of the spins resulting from occupied d_{xy}-orbitals at checkerbosard arranged Ti^{3+}-sites. Electron hopping on a 50% occupied Ti-sublattice (a quarter-filled band) and/or lattice relaxations are discussed as origin of the measured conductivity.

(submitted to: Phys. Rev. B, (in press))
Contact person: Rossitza Pentcheva (pentcheva@lrz.uni-muenchen.de)

All-electron study of InAs wurtzite: structural and electronic properties

Zeila Zanolli and Ulf von Barth
Department of Physics, Lund University,
Sölvegatan 14 A, 223 62 Lund, Sweden

Abstract

The structural and electronic properties of the wurtzite phase of the InAs compound are, for the first time, studied within the all-electron Density Functional (DF) approach. We used the full-potential linearized augmented plane wave (LAPW) method within the local density approximation (LDA) for the exchange-correlation potential. From the structure optimization of the wurtzite polymorph it was found that the c/a ratio is somewhat greater than the ideal and that the internal parameter u has the ideal value. The wurtzite polymorph has a smaller equilibrium volume per InAs pair and a lower binding energy when compared to the zinc-blende phase, hence confirming the zinc-blende as the stable polymorph. The influence of the relativistic effects on the band structure is investigated. The bands are calculated within a non-relativistic and a scalar-relativistic approach including or not including Spin-Orbit interaction. We find that the energy gaps of both polymorphs are positive when obtained from a non-relativistic calculation and negative otherwise.

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Contact person: zeila.zanolli@ftf.lth.se

GW band structure of InAs and GaAs in the wurtzite phase

Z. Zanolli
Department of Physics, Lund University,
Sölvegatan 14 A, 223 62 Lund, Sweden
J. Furthmüller
Institut für Festkörpertheorie und optik, Friedrich-Schiller-Universität,
Max-Wien-Platz 1, 07743 Jena, Germany
F. Fuchs
Institut für Festkörpertheorie und optik, Friedrich-Schiller-Universität,
Max-Wien-Platz 1, 07743 Jena, Germany
U. von Barth
Department of Physics, Lund University,
Sölvegatan 14 A, 223 62 Lund, Sweden
F. Bechstedt
Institut für Festkörpertheorie und optik, Friedrich-Schiller-Universität,
Max-Wien-Platz 1, 07743 Jena, Germany

Abstract

We report the first calculations of the quasiparticle structure of a newly observed polymorph of InAs and GaAs, i.e., the wurtzite phase. The calculations are performed in the GW approximation using plane waves and pseudopotentials. For comparison we also report the study of the zinc-blende phase conducted within the same approximations. In the InAs compound the In 4*d* electrons play a very important role: whether they are frozen in the core or not, leads either to a correct or a wrong band ordering (negative gap) within the Local Density Appproximation (LDA). We have calculated the GW band structure in both cases. In the first approach, we have estimated the correction to the *pd* repulsion calculated within the LDA and included this effect in the calculation of the GW corrections to the LDA spectrum. In the second case, we circumvent the negative gap problem by first using the screened exchange approximation and then calculating the GW corrections starting from the so-obtained eigenvalues and eigenfunctions. This latter more fundamentally correct approach leads to a more realistic band-structure. Thus, this approach was also used in the GaAs compound leading to better results as compared to the traditional way of perturbatively adding GW corrections to the LDA band structure.

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Contact person: zeila.zanolli@ftf.lth.se

Magnetic order and valency at $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ interfaces

H. Zenia
Department of Physics and Astronomy, University of Sheffield,
Sheffield, S3 7RH, UK
and Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK
G. A. Gehring
Department of Physics and Astronomy, University of Sheffield,
Sheffield, S3 7RH, UK
W. M. Temmerman
Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK

Abstract

We report on first principles calculations of the electronic structure of $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ junction with two possible types of interface terminations. We find that the $La_{0.7}Sr_{0.3}O/TiO_2$ interface preserves the interlayer ferromagnetic coupling between the interface MnO_2 layer and the bulk. The other interface, MnO_2/SrO, favours antiferromagnetic coupling with the bulk. By inserting two unit cells of undoped $LaMnO_3$ at the interface the ferromagnetism is recovered. This is understood in terms of the doping level and the mobility of carriers near the interface.

(cond-mat/0604343)
Contact person: H.Zenia@sheffield.ac.uk

7 Presenting Other Initiatives

7.1 Master's Program in Computational Science, Frankfurt/M

New Master's Program *Computational Science*
at J.W.Goethe-Universität Frankfurt am Main

In response to the increasingly important role played by large-scale numerical simulations in science and engineering, as well as business, economics, financial markets and medicine, J.W.Goethe-Universität Frankfurt has established a new Master's program *Computational Science*, which will start in October 2006. The primary goal of this two-year program is training students in the natural sciences for computer-based research and development. The program targets outstanding students with a Bachelors degree in Biology, Chemistry, Geoscience or Physics, but is equally open to exceptional students with a degree in Mathematics, Computer Science or Engineering who also have a solid background in one of the natural sciences. Building on the common platform of mathematical and methodological expertise acquired during the Bachelors studies, the Master's program leads students towards the current state-of-the-art of research, both with respect to their specific field within the natural sciences and with respect to computational techniques. The program covers both the basic tools for numerical simulation, provided by applied mathematics and computer science, and the formulation of efficient, yet realistic models in the individual disciplines, which requires an understanding of the scales, interactions and correlations involved.

The M.Sc. in *Computational Science* is administered jointly by the Departments of Biochemistry, Chemistry and Pharmacy, Geoscience / Geography, Physics as well as Computer Science and Mathematics, together with the Frankfurt Institute for Advanced Studies and the Center for Scientific Computing. These Institutions encompass a wide variety of fields, including

- Biochemistry, Chemformatics, Molecular Dynamics, Quantum Chemistry
- Elementary Particle Physics, Heavy-Ion Physics, Condensed Matter Theory, Soft Matter
- BioNanoscience, Theoretical Biology, Neuroscience
- Meteorology, Hydrology, Mineralogy, Geodynamics
- Distributed Systems, Parallel Computers, Computer Graphics, Design Methodology
- Numerics of Dynamical and Controlled Systems, Stochastical Differential Equations, Optimization

The structure of the curriculum is highly interdisciplinary: Rather than providing separate routes to graduation for the individual disciplines, its modules are designed to allow students to cross disciplinary boundaries as they choose. The resulting education fosters research and development at the interfaces between the traditional fields and strengthens interdisciplinary communication. Particular emphasis is placed on individual research. A student's thesis project will directly address an open question at the forefront of science. Students are fully integrated into research groups during both the training phase as well as during their individual thesis work. The working language of the entire M.Sc. program is English, consistent with the international background of our students.

A complete overview of the program can be found at:

http://www.physik.uni-frankfurt.de/mpcs/

Please refer to this page for information regarding admission requirements, the selection of students, the application procedure and the curriculum. For additional information please contact:

Dr. Eberhard Engel
Address: Center for Scientific Computing
J.W.Goethe-Universität Frankfurt am Main
Max-von-Laue-Str. 1
D-60438 Frankfurt am Main
Germany
Phone: (++49) 69 - 798 47351
FAX: (++49) 69 - 798 47360
E-mail: engel@th.physik.uni-frankfurt.de

7.2 Introductory Graduate Class on Atomistic Modeling of Materials

Gerbrand Ceder and myself have recently prepared an introductory graduate class on atomistic modeling of materials. This is now freely available on the web at

http://ocw.mit.edu/OcwWeb/Materials-Science-and-Engineering/3-320Spring-2005/CourseHome/index.htm

The class follows GNU GPL guidelines, and so all the material is available, copyright-free, for use and/or redistribution.

The class includes video lectures, lectures slides, homework assignments and solutions, and covers basic principles of classical and electronic-structure modeling, with a specific focus on materials applications. It is generally suitable for students that have no prior experience in the field, and it is based on freely available or open-source software, such as GULP or Quantum-Espresso.

Any feedback on the class will also be greatly appreciated - this is a work in progress that will be revised in future years.

We would also be grateful if you were to link the class from relevant websites.

Prof Nicola Marzari
Department of Materials Science and Engineering
13-5066 MIT
77 Massachusetts Avenue
Cambridge MA 02139-4307
USA
E-mail: marzari@mit.edu
http://quasiamore.mit.edu

8 SCIENTIFIC HIGHLIGHT OF THE MONTH: "Infrared spectrum of hydrous minerals from first-principles calculations"

Infrared spectrum of hydrous minerals from first-principles calculations

Etienne Balan[1,2], Michele Lazzeri[2], Francesco Mauri[2]

[1] IRD- UMR 161 CEREGE, Europole Méditerranéen de l'Arbois
BP 80, 13545 Aix en Provence cedex, France,
[2] Institut de Minéralogie et Physique des Milieux Condensés (IMPMC), UMR CNRS 7590,
Universités Paris VI et VII, IPGP, 4 Place Jussieu, 75252 Paris Cedex 05, France.

Infrared spectroscopy is widely used to determine and investigate the structure of the finely divided mineral phases, which typically form in soils and weathering environments [1]. It provides information ranging from the detection and identification of specific or minor mineral constituents, hardly accessible from X-ray diffraction techniques, to the determination of the stacking order and ordering pattern of substituting cations in clay minerals [2, 3]. Other applications include the mineralogical quantification in complex samples [4], the detection of mineral transformations in geological environments [5] and the investigation of the interfacial properties of minerals, through the adsorption of probe molecules [6]. Infrared spectroscopy can be performed using a large variety of experimental geometry. Concerning powder minerals, most of the spectra are recorded in the transmission mode through a rigid disk containing the powder particles diluted in a homogeneous non-absorbing matrix, such as KBr. However, other configurations can be used, such as diffuse reflectance for powdered materials [7] or attenuated total reflectance to investigate the interface between solids and aqueous solutions [6]. In complex natural samples, spectra may also be recorded from thin sections using infrared microscopy techniques [8].

The straightforward interpretation of vibrational infrared or Raman spectra is often difficult, in particular when considering finely divided and poorly ordered minerals, such as clays. On the one hand, it is experimentally difficult to measure the polarization properties of very fine particles. On the other hand, there is not always an evident relation between the microscopic atomic structure and measured vibrational bands. An additional complexity of powder spectra also arises from the influence of the shape of particles on the vibrational spectra. In fact, in polar insulators, atomic vibrations can be associated with oscillating macroscopic electric fields that are determined by the macroscopic shape of the particles. Because of all these reasons, a theoretical determination (independent from the experiment) of the vibrational frequencies and intensities is an ideal tool to establish unambiguous relationship between the vibrational spectrum and the microscopic structure of minerals. In this context, the use of very precise first-principles computational methods based on density functional theory is extremely useful [9]. In a polar insulator, the vibrational spectrum can be obtained knowing the analytical part of the dynamical matrix and dielectric quantities such as the Born effective charges and the electronic dielectric tensor [9, 10]. These quantities can be calculated as the second-order derivatives of the total energy with respect to atomic displacements and/or an external uniform electric field, using the linear response theory [9]. Finally, the dependence of the vibrational spectroscopic properties on the dielectric properties is determined by the macroscopic shape of the considered system. Combining first-principles calculations of crystal properties with a model taking into account experimental and sample-dependent parameters, it is possible to significantly improve the comparison between theory and experiment, going a step beyond the simple comparison of the eigen values of the dynamical matrix with experimental band positions.

As a first attempt, we have investigated the infrared spectrum of kaolinite which displays well-resolved absorption bands [11]. The structure of kaolinite has been extensively investigated by neutron and X-ray powder diffraction (e.g. Ref. [12]). IR spectroscopy was also extensively used to investigate the hydroxyl groups and H-bonding pattern in kaolinite [1,2,13,14]. The structure of kaolinite-group minerals is formed by a stacking of 1:1 layers (Fig. 1). Each layer contains a pseudo-hexagonal silica sheet of corner-shared SiO_4 units linked to a dioctahedral sheet of edge sharing $AlO_2(OH)_4$ octahedra. Two kinds of OH groups can be distinguished. The inner-surface OH groups, which are located at the top of the dioctahedral sheet, are hydrogen-bonded with the basal plane of oxygen atoms of the next layer. Other OH groups (inner OH groups) are located inside the layer, between the dioctahedral and tetrahedral sheets, pointing horizontally toward the center of the ditrigonal cavity. Using the structure determined by Ref. [12] as an initial guess, an excellent agreement between the experimental and theoretically relaxed structure was obtained. The infrared spectrum derived from this theoretical structure is in very good agreement with its experimental counterpart (Fig. 1). A simple comparison between experiment and theory makes it possible to assign the IR bands to vibrational mode. For example, in the range of the OH stretching vibrations (Fig. 2), the band experimentally observed at 3620 cm^{-1} corresponds to the inner OH stretching. The one observed at 3695 cm^{-1} corresponds to the in-phase motion of the three inner-surface OH group, whereas the bands at 3669 cm^{-1} and 3652 cm^{-1} correspond to the out-of-phase motion of the inner-surface OH groups. This interpretation, based on coupled vibrations of neighboring OH groups, is consistent with the assignment given by Refs. [1, 14]. The previously suggested one-to-one correspondence between an IR band and a single OH group [15] is thus disproved.

The experimental position of OH stretching bands is reproduced within 1% by calculations performed using the harmonic approximation. This apparently good accuracy is however not consistent with the large anharmonicity of OH vibrations inferred from the vibrational frequency of isotopically exchanged materials [16] or from the frequency of overtones observed in the near infrared range [17]. In fact, the theoretical anharmonicity constant related to the stretching of the inner-OH group of kaolinite is -95.2 cm^{-1}, which is consistent with the experimental value of -86.5 cm^{-1} deduced from the frequency of the first overtone bands [17]. The very

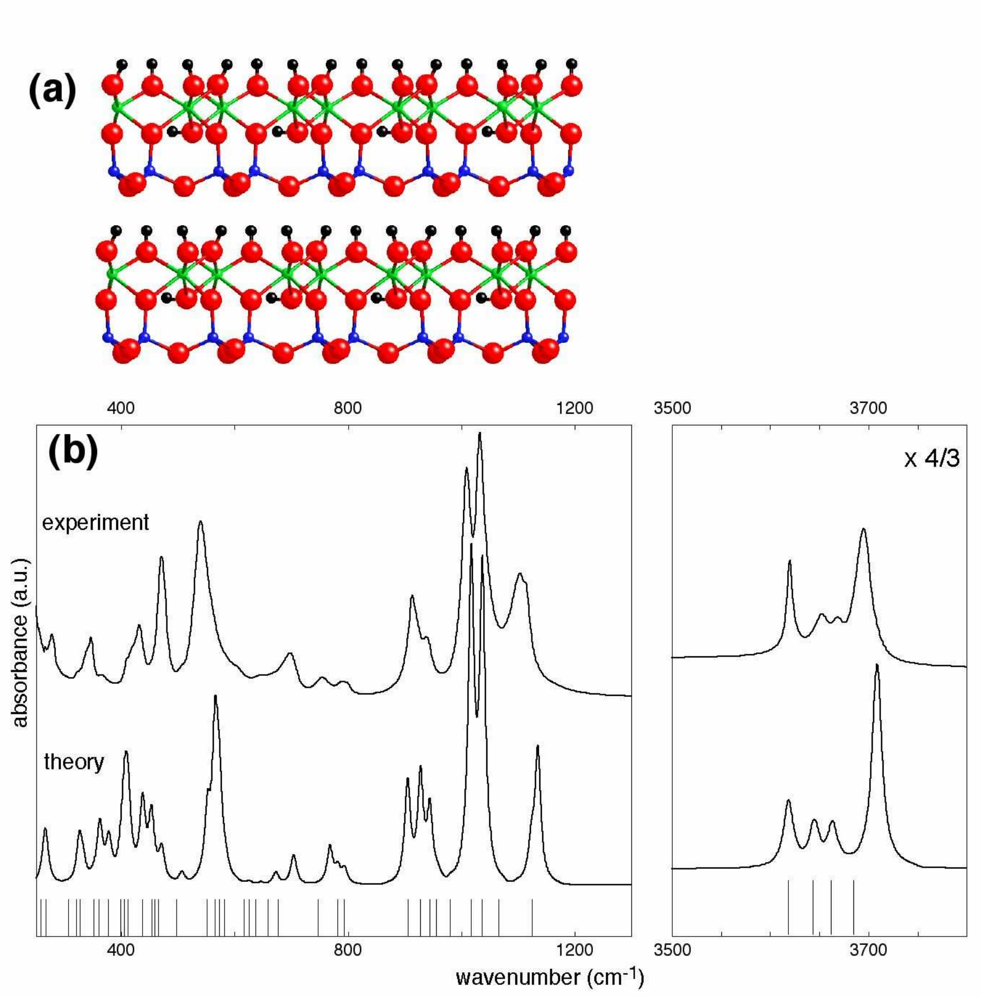


Figure 1: (a) View of the kaolinite structure showing the stacking of two layers. Note the inner-surface and inner OH groups with orientation perpendicular and parallel to the layer, respectively. (b) Theoretical and experimental infrared spectrum of kaolinite. Vertical bars correspond to the phonon frequencies. Note the very good agreement between theory and experiment making it possible to assign the absorption bands in terms of vibrational modes.

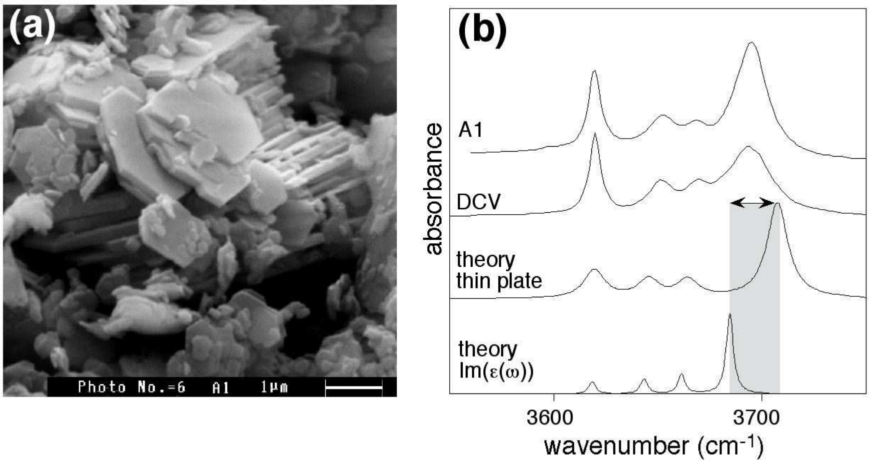


Figure 2: (a) Scanning electron micrography of a well-ordered kaolinite sample (sample A1). Note the platy shape and micrometric size of the particles. (b) Infrared spectrum of a fine (A1) and coarse (DCV) sample of kaolinite. The coarse kaolinite sample displays a significant broadening of the high frequency band. The theoretical spectrum calculated for a thin platy particle shape displays a significant shift of this band with respect to the resonances of the imaginary part of the dielectric tensor ($\mathrm{Im}(\epsilon(\omega))$), computed for a zero macroscopic electric field. For any other particle shape, the high-frequency band would occur within the shaded area; which explains the broadening observed in the coarser sample.

good agreement obtained between absolute frequencies derived from harmonic calculations and experimental frequencies thus results from the cancelation of errors related to the approximations used in DFT calculations and to the neglect of anharmonicity [18].

Further theoretical investigations have been performed on minerals displaying larger unit cell size and more complex vibrational structure. These minerals include dickite and nacrite, the polymorphs of kaolinite [19], and gibbsite, an Al hydroxide commonly found in lateritic and bauxitic formations [20]. Their structure can be described as a regular stacking of 2-layers units, each layer being related to the adjacent one by a glide plane. In the three cases, the theoretical modeling of infrared spectra enabled an unambiguous assignment of OH bands in terms of vibrational modes (see Fig. 3 for gibbsite). These investigations have shown that a significant coupling of the OH motion occurs not only between neighboring OH groups, but also between adjacent layers for the modes polarized perpendicularly to the layers. This unexpected observation underlines the long-range character of electrostatic interactions and the importance of accurate modeling tools to interpret the infrared spectra of minerals.

Effects related to long-range electrostatic interactions may occur not only in the IR spectra of structures based on 2-layers units but also in that of any fine-grained minerals, with a particle size smaller than the wavelength of the IR light (i.e. 3 μm). For example, the powder infrared spectrum of kaolinite reveals subtle relationships between the morphology of particles and their vibrational properties [14, 21]. Kaolinite particles indeed often display a platy shape, the basal plane of the plates being parallel to the dioctahedral layers (Fig. 2). In that case, the displacement of electrostatically charged ions perpendicularly to the layers creates a surface charge on each side of the particle, which behaves as a condensator. The surface charge induces

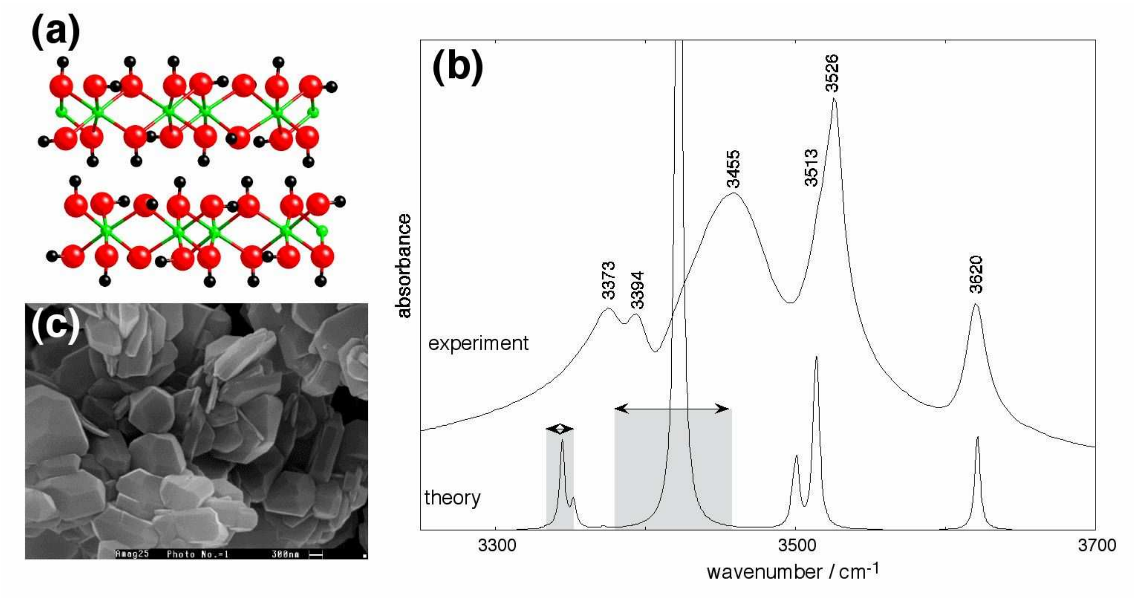
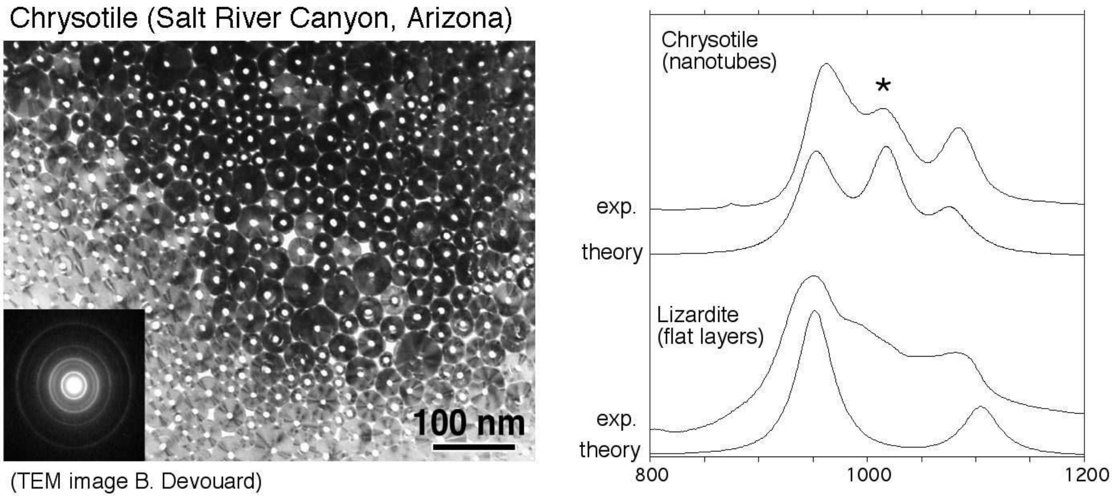


Figure 3: (a) View of the gibbsite structure (α-Al(OH)$_3$) showing the stacking of two layers. Note that OH groups may have an orientation perpendicular or parallel to the layer. (b) Scanning electron micrography of a synthetic gibbsite sample with equant particle shape. (c) Comparison between the experimental and theoretical powder spectra of gibbsite in the range of OH stretching vibrations. The theoretical spectrum has been calculated for a spherical particle shape. Depending on the shape of gibbsite particles, intense bands polarized perpendicularly to the layers may occur within the shaded zones, explaining their significant broadening.



(TEM image B. Devouard)

Figure 4: (a) Transmission electron micrograph of the investigated chrysotile sample (Phillips Mine, Salt River Canyon, Arizona), section perpendicular to the fiber axes. Inset: selected area electron diffraction pattern showing the parallel texture of chrysotile fibers seen along [100]. (b) Transmission powder IR absorption spectra of chrysotile and lizardite in the range of Si-O stretching bands. The theoretical spectrum of chrysotile has been computed by assuming that the chrysotile tube is a dielectric continuum, locally identical to lizardite. The comparison with experiment shows that the additional band observed in the chrysotile spectrum (star) is not related to a microscopic distortion of the structure but to collective charge excitations due to the peculiar electrostatic properties of multiwall chrysotile nanotubes.

a macroscopic electric field opposing the displacement of ions. Compared to an infinite crystal, a higher energy is thus required to displace the ions. Such increase corresponds to a higher vibrational frequency, leading to a significant blue-shift of the absorption bands. Theoretical calculations provide a quantitative modeling of this phenomenon in excellent agreement with experimental observations. For example, in the range of the stretching OH modes of kaolinite, the high frequency absorption band is related to the in-phase motion of inner-surface OH groups perpendicularly to the layers. Depending on the sample, this band may present a significant broadening, which is not related to a decreasing crystal order. Indeed, among two well-ordered samples, the broader band is observed in the most ordered one, which also displays a larger grain size (Fig. 2). In fact, theoretical calculations show that this band is shifted by ~ 20 cm^{-1} between an infinite crystal and a thin plate of kaolinite. The thin plate geometry corresponds to the maximum shift of this band because the polarization of the corresponding vibrational mode is perpendicular to the plate. The broadening of the band therefore arises from the sensitivity of the band frequency to the particle shape, taking into account that different shapes always coexist in a given powder sample. Similar phenomena have been observed in the IR spectrum of gibbsite, which displays a strong dependence on the particle shape [22]. For a sample with relatively equant particles (Fig. 3), the best agreement between theory and experiment is obtained by considering the theoretical spectrum of spherical particles. It is noteworthy that only intense bands are significantly affected, which produces intense and broad features in the experimental spectra. The broadening is related not only to the occurrence of particles with different shape in a given sample but also to the inhomogeneity of the macroscopic electric field induced in particles whose shape differs from that of a perfect ellipsoid.

More complex effects can be observed for specific particle shapes. Particularly interesting is the case of serpentine minerals which display platy or tubular morphologies in lizardite and chrysotile, respectively (Fig. 4). Theoretical investigations have shown that the peculiar electrostatic properties of the chrysotile nanotubes leads to unexpected additional vibrational bands in the IR spectrum of chrysotile, compared with that of lizardite [23–25]. This shape-effect explains the differences recognized a long time ago between the infrared spectrum of serpentine polytypes [26] and gives a characteristic infrared signature to determine the presence of chrysotile asbestos in composite materials.

Finally, we would like to stress the importance of calculating both frequency and intensity to reach an unambiguous interpretation of the infrared spectrum of minerals. Because of the intrinsic theoretical uncertainty of mode frequency (within a few relative percents), the computation of the eigen values of the dynamical matrix only is generally not sufficient to perform a one-to-one assignment of experimental bands. In addition, the calculation of spectral intensities provides an easy way to compare theory with experiment, making the result of theoretical calculations more accessible to experimentalists.

Calculations were performed at the IDRIS institute (Institut du Développement et des Ressources en Informatique Scientifique) of CNRS (Centre National de la Recherche Scientifique) using the PW and PHONON codes (http://www.pwscf.org).

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