Ψ_k Newsletter

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

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Contents

1 Editorial

In this newsletter we announce several postdoctoral positions associated with a new Research Training Network on f-electron Physics (RTN2), and they can be found in the section dedicated to this new RTN2. Moreover, in the section of the last remaining TMR Network ("Psi-k"), coordinated by Axel Svane (Denmark), there is the fourth annual report on the scientific activity of this network in the past year. In this newsletter readers will also find four reports on workshops organized within the RTN1 on 'Magnetoelectronics' (one) and the ESF Psi-k Programme (three). Note that three of them concern 'hands-on computer code' workshops, and two contain abstracts of presented papers. In the **News from the ESF Programme** we also have one report on a collaborative visit, and several workshop announcements. Most important in this section are, however, a call for proposals for workshops in 2003, as well as, a call to join one of the 15 working groups in the new ESF Programme. Please do take time and give some consideration to those calls. In the same section we also have a report by the Psi-k 'consultant' on the first CECAM Advisory Committee, which may be of relevance for future stronger links between the Psi-k and CECAM. The general workshop/conference and job announcements are placed in the two sesctions following the **ESF Programme** section. Abstracts of newly submitted papers are in the usual **Abstracts** section. The scientific highlight is by Iosif Galanakis, the RTN1 postdoctoral fellow with the Juelich partner of this network. The title of the highlight is **"Half-ferromagntism and Slater-Pauling behaviour in the Heusler alloys"**. Please check the table of contents for further details.

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

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

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

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

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

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

Dzidka Szotek and Walter Temmerman
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2 News from the Research Training Network on Magnetoelectronics (RTN1)

COMPUTATIONAL MAGNETOELECTRONICS

2.1 Reports on RTN1 Workshops

2.1.1 Report on Hands-on KKR and Spectroscopies Course

University of Munich, 19-22 February 2002

The first ever hands-on course on the KKR method took place in München 19-22 February 2002. It welcomed 32 participants and 14 lecturers (list of participants and lecturers included).

The KKR method is notoriously difficult to automate due to the energy dependence of the KKR matrix and the free electron solutions of the KKR structure constants. However this was accomplished by the Munich SPR-KKR (spin polarized relativistic Korringa-Kohn-Rostoker) program package

(see http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/SPRKKR/).

The package is more versatile than producing bands, densities of states, total energies etc. and incorporates a staggering amount of spectroscopy calculations such as XANES, EXAFS, magneto-optics, angle integrated photoemission, auger electron spectroscopy and compton scattering. The codes can be run in a non-relativistic and relativistic manner and contain sufficient tools to analyse the effect of the spin-orbit interaction. Moreover, the package can treat ordered and disordered alloys and magnetic multilayers. Included in the package are many tools to analyse the electronic structure such as phase shift plots. All of this was embedded into an easy to use multi purpose Graphical User Interface (GUI) called XBAND

(see http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/xband.html).

Actually, the XBAND feature was most popular with the experimentalists. Set exercises for four afternoons were available giving the participants the opportunity to acquaint themselves with all features of performing electronic structure and spectroscopy calculations. The participants were also given the opportunity to investigate systems of their own interest and systems such as $ZrZn_2$, NiO, $Cu_{0.95}Ni_{0.05}$ were also studied.

A well balanced series of lectures (some lecture notes can be found under:

http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/Hands-onCourse/)

accompanied the practical hands-on sessions: the fundamentals of the KKR and the use of the XBAND package and KKR code were taught by Walter Temmerman and Hubert Ebert, respectively. Three experimental spectroscopy talks emphasised the relevance of this course to X-ray absorption spectroscopy (K. Baberschke), X-ray magneto-optics (Ch. Mertins) and photoemission (C.M. Schneider). The basics of DFT and one-electron theory of spectroscopies were reviewed by Engel and Strange, respectively. More advanced topics, which also highlighted applications of the codes, included relativity in electronic structure calculations (B.L. Gyorffy), GW treatment of excited states (A. Schindlmayr), CPA (I. Turek), surface magnetism (L. Szunyogh), temperature dependent magnetism (J. Kudrnovsky) and magnetoelectronics (P. Dederichs).

The course succeeded in teaching the basics of performing KKR and spectroscopy calculations and giving the participants a deeper understanding in the KKR and Green's function methods. We foresee that in the near future the Munich SPR-KKR program package will further increase its functionality in particular through the incorporation of more spectroscopies.

Hubert Ebert and Walter Temmerman

Introduction to bandstructure calculations: KKR method

Walter Temmerman

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A short introduction is given to the KKR method. This covers a formal definition of the Green's function and its properties. Then, using the Green's function, the scattering formalism is developed for free space and for the single site, allowing for the introduction of phase shifts. The importance of the phase shifts in the analysis of the electronic properties is stressed. The theory of multiple scattering is then written down with concepts such as the scattering path operator. Recent developments such as screening are derived. Finally, a summary of the advantages and disavantages of the KKR method with respect to other bandstructure methods is given.

The Munich SPR-KKR code

H. Ebert

University of Munich

The talk gives a short introduction to the functionality and formal background of the Munich spin-polarised relativistic (SPR-KKR) program package (see

http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/SPRKKR/).

First, in short the various available calculation modes, the electron structure information that can be obtained and the various kinds of electronic spectroscopy that can be studied are surveyed.

Presenting the formal background of the SPR-KKR package emphasise is laid on the fully relativistic mode for magnetic solids. Technical details connected with that as for example the coupled radial Dirac equations, the single site t-matrix, symmetry considerations are discussed in some detail. Two ways to determine the so-called scattering path operator are explained: The real space cluster mode is used for high energies (EXAFS) and to deal with surfaces at the moment. The Brillouin zone integration technique, on the other hand, is used as the standard method for most other purposes. Using this technique exploiting symmetry is indispensable. The simultaneous presence of spin-orbit coupling and spin magnetisation, however, has rather important consequences for this as it is demonstrated. An important feature of the program package is the ability to deal with disordered systems by using the CPA (Coherent Potential Approximation). The basic ideas of he CPA are described and its implementation within the KKR-method is outlined. Finally, a short outlook on future developments is presented.

Density functional theory for magnetic solids

E. Engel

J.W.Goethe Universitaet Frankfurt

In the talk an overview of the foundations of density functional theory is given. After a discussion of the Hohenberg-Kohn theorem the kinetic energy functional of noninteracting particles (T_s) and the crucial exchange-correlation (xc) energy functional (E_{xc}) are introduced. Assuming the existence of a noninteracting system with the same density as the interacting system of interest, one can establish the Kohn-Sham equations, thus ensuring an exact treatment of T_s. As the most simple approximation for E_{xc} the local density approximation (LDA) is presented. The extension of the complete formalism to spin-density functional theory, which is required for studying magnetic systems, is also discussed. On this basis it is shown that the LDA yields fairly accurate results for the properties of simple metals but fails to predict the correct ground state of iron. Thus, finally, the concept of the generalized gradient approximation is briefly reviewed, which resolves some of the deficiencies of the LDA (as e.g. the problem with iron).

X-ray Absorption Spectroscopy: Magnetism in Thin Films

K. Baberschke

Freie Universität Berlin

The X-ray Absorption Spectroscopy is a technique in which the absorption coefficient μ(E) is measured as function of incoming photon energy. This is compliment ary to the photon electron spectroscopy at which the energy of the outgoing photon electron is analyzed. XAS is a widely used technique in all kinds of material research. Using circular polarized synchrotron radiation it can be used to study magnetic properties by means of x-ray magnetic circular dichroism

(XMCD). This lecture covers four topics in which the magnetism of 3d, 5d and 4f magnetism is investigated:

1.Magnetic circular dichroism at Vanadium. Using the new facility BESSY II we present XMCD spectra for a trilayer of Fe/V/Fe, noise-free and of excellent quality. Several detailed features of the XMCD at the L3,2 edges are discussed. This remains a challenge for theoretical interpretation because the commonly used sum rules cannot so successfully be applied for elements at the beginning of the 3d series (collaboration with H. Ebert, LMU).

2.Induced magnetism for Fe/W Orbital and Spin Magnetic Moments. For an Fe/W interface we have investigated at ESRF, Grenoble, the induced magnetism at the Tungsten interface in the hard x-ray regime. This induced moment at W is oriented anti-parallel to magnetization of Fe and the orbital momentum of W is aligned parallel to its spin moment. This is a surprise and was not found in bulk alloys. Details are published in PRL 85, 413(2000).

3.Quadrupolar contributions in XMCD: Tb-metal E2/E1. Again at the ESRF in the hard x-ray regime we have observed quadrupolar and dipolar transitions at the L3,2 edges of 4f elements. Using SCF real space full multiple sketching theory, we were able to separate the dipolar and quadrupolar contributions. Details will be published in H. Wende et al. JPA 91, XXX 15. Mai 2002.

4.Magnetic EXAFS: Example 1 - 3 and most of the literature discusses the XMCD only in the near-edge regime of the L and K edges respectively. It should be noted that the dichroic signal extends over a large range in energy, and a so-called "spin-polarized EXAFS" can be detected. The temperature dependence of the amplitude for normal EXAFS is usually discussed in terms of a Debye-Waller-factor. For the spin-polarized EXAFS in analogy the temperature-dependent damping can be interpreted in terms of spin fluctuations. In contrast to neutron scattering EXAFS allows to separate nearest neighbor from next nearest neighbors effect. Examples of local spin fluctuations for Fe, Co, Gd are given in: H. Wende et al., J.Synchrotron Rad. 8, 419 (2001)

One Electron Theory of Spectroscopies

P. Strange

Keele University, UK

In this talk I discussed time-dependent perturbation theory and its applications in understanding spectroscopies. The lecture started with a brief description of the first and second order golden rule for calculating transition rates. After this was a description of how we calculate the various quantities that go into the golden rule. Firstly we discussed the photon and how it is described within quantum field theory as a quantised vector potential. This forms the perturbation in the theory. Following this I showed how to build up the matrix elements in the golden rule and how to evaluate the photon part of those matrix elements. This enables us to reduce the description of spectroscopies to a single-particle-like problem. We then have to decide how to describe the electron system and this is done using density functional theory and the multiple scattering approach to electronic structure discussed by other lecturers in this workshop. The next step was to explain how the matrix elements in the golden rule can be written in terms of the scattering Green's function. Theoretical expressions for the transition rate were then written down and discussed for X-ray absorption and emission, valence band photoemission, Auger electron spectroscopy and X-ray scattering. There was also a brief discussion of synchrotrons and the polarisation of x-rays and of how appropriate the single-particle picture of spectroscopies really is. The role of the self-energy in modifying the spectra calculated within the single-electron-like theory was also discussed. Throughout the lecture the advantages and disadvantages of both relativistic and non-relativistic theory were emphasised and described. I demonstrated that spectroscopy is an excellent meeting point for theory and experiment and that such experiments form a good testing ground for our theories of electronic structure. However, it was emphasised that basing a theory of spectroscopy, which involves excitations of the electron system, on density functional theory which rigorously is a theory of the ground state of the electrons only, is not entirely satisfactory and means that we can only really justify the theory in retrospect. I hope that the lecture demonstrated that the combination of time-dependent perturbation theory and density functional theory implemented using multiple scattering theory provides a straightforward and succinct theory of spectroscopies.

The coherent potential approximation for random alloys - theory and applications

I. Turek

Institute of Physics of Materials AS CR, Brno & Charles Univ. Prague

The lecture introduces the single-site coherent potential approximation (CPA) for an efficient description of substitutionally disordered alloys. The theory is illustrated by calculations of selected electronic properties of spin-polarized systems. Following topics are included:

i) Introduction to the random alloys: general concepts and the CPA in semiempirical tight-binding and ab initio (KKR) methods.

ii) Bulk alloys: spin-dependent disorder in binary magnetic alloys, concentration dependence of magnetization, the Invar effect in alloys.

iii) Alloy surfaces and metallic interfaces: magnetization at alloy surfaces, interface interdiffusion and exchange coupling.

iv) The disordered local-moment state: paramagnetic state of transition metals, local moment disorder in metallic spin glasses and in diluted magnetic semiconductors.

v) Interatomic interactions in alloys: interplay of magnetism and chemical interactions, the Ising hamiltonian for binary alloys.

RELATIVISTIC EFFECTS IN THE ELECTRONIC STRUCTURE OF SOLIDS

B. L. Gyorffy

H.H. Wills Physics Lab., University of Bristol, UK

Even if a piece of metal is stationary, electrons on the Fermi Surface may move with velocity, v_F, compared to that of light, c. Thus, in describing the electronic structure of solids relativistic effects will have to be taken into account. An efficient way of doing this is to describe them by the Dirac equation. The first part of the talk was an account of what such description entails in the Korringa-Kohn-Rostoker (KKR) approach to solving the relativistic Kohn-Sham equations to Density Functional Theory (DFT) for electrons in condensed matter. This introduction was followed by brief discussions of a few representative examples of physical phenomena, which critically depend on relativistic effects playing a role.

The first example was the yellow colour of solid gold (Au). This was explained as the indirect effect of the relativistic contraction of the atomic core on the $5d - 6s$ optical transition. The next one concerned the thickness of Bloch Walls between magnetic domains in bcc iron (Fe). Here the relativistic effect was the magneto-crystalline anisotropy, which is due to the coupling of the electronic spin and the orbital degrees of freedoms. As an illustration of how it comes about the recent first-principle calculation of a 90 Bloch Wall in bcc iron by Schwitalla et al. [PRB, 2001] was briefly reviewed. Finally the first-principles calculations of the magnetocrystalline energies of linear Fe chains, with various orientations, embedded in fcc Cu was discussed. It was argued that the surprisingly large anisotropy energies of these very asymmetrical structures may be of technological importance in fabricating hard magnets.

Soft X-Ray Magneto-Optical Polarization Spectroscopy

H.-Ch. Mertins

BESSY Berlin

Magneto-optical (MO) spectroscopies can be classified into intensity measurements like the commonly used X-ray magnetic circular dichroism (XMCD) and polarization experiments. The second class, is based on the relatively new technique of soft X-ray polarization analysis, exploiting the polarizing properties of multilayer optics /1/. The advantage of the polarization analysis over an intensity measurement is the knowledge of the polarization state of light after its interaction with the sample, i.e. the intensity and the phase. This in turn directly yields completely the optical constants which gives the full description of the interaction between polarized light and magnetic matter making possible a separation between pure magnetic and non-magnetic charge effects. In this way the X-ray Faraday effect was investigated at BESSY /2/ and the experimental data proved the validity of ab-initio calculations /3/.

Recently we observed the Voigt effect, a new X-ray MO phenomenon that is, in contrast to the XMCD and Faraday effect, quadratic in the magnetization M /4/. The Voigt effect is observed with linearly polarized light. After passing a magnetized foil, the plane of polarization is rotated by an angle qV and it is changed to elliptical, as expressed by its ellipticity tan(eV). Both are detected by a polarization analysis of the transmitted light. We observed a maximum rotation value of up to 7.5 deg./mm which is almost an order of magnitude larger than that observed in the visible. The Voigt rotation was found to be independent of the magnetization direction, as theoretically expected, demonstrating the quadratic magnetic response. Further, our ab-initio calculations agree with the experimental results and show that the X-ray Voigt effect critically depends on the core spin splitting, although the spin splitting of the 3/2, -3/2 sublevels of Co is only 0.79 eV.

Thus, combined with ab-initio calculations, the X-ray Voigt effect provides a powerful new instrument to investigate the core polarization. Its dependence on the square of the magnetization opens up new ways to study antiferro magnetic materials on an element selective level. Support by the Euro. Comm. (ERBFMGECT980105), BMBF (05KS1IPB/8) and SFB 463, Dresden.

1 F. Schäfers et al., Appl. Opt. 38, 4074 (1999)
2 H.-Ch. Mertins et al., Phys. Rev. B 61, R874 (2000)
3 J. Kunes et al., Phys. Rev. B 64, 174417-1 (2001)
4 H.-Ch. Mertins et al., Phys. Rev. Lett. 87, 047401-1 (2001)

Calculation of Electronic Excitation Spectra

P. Strange

Keele University, UK

In this talk I discussed the relativistic theory of valence band photoemission in detail. The starting point was the formal expression for the photocurrent discussed in my previous lecture. I showed how to rewrite the photocurrent in a computationally convenient form. Some technical points about the implementation were described, particularly the origin of the selection rules and their dependence on the polarisation of the photon. In the second half of the talk I went on to discuss how the photoemission spectra can be interpreted in terms of the band structure of materials. I showed that it can be used to map out individual energy bands. With this possibility angle-resolved photoemission is a very sensitive test of our theory of electronic structure. I also showed how we could take advantage of the polarisation of the incident photon and the spin of the emitted electron to use photoemission to measure exchange splittings, spin-orbit splittings and as a measure of magnetic anisotropy energies. Throughout the talk it was emphasised that we interpret the spectroscopy in terms of the one-electron like energies of density functional theory (DFT). However these are really just Lagrange multipliers within DFT introduced to maintain normalisation. We should always realise that agreement between such a theory and experiment is close to miraculous.

Surface Magnetism

L. Szunyogh

Budapest University of Technology and Economics & Vienna University of Technology

In general, Surface Magnetism covers a wide area of research activity extending from the investigation of surfaces of magnetic metals and alloys, ultrathin magnetic films, through more complicated structures like bilayers, trilayers and multilayer systems to artificially manufactured nanostructures like magnetic dots and quantum corrals. Many novel, surprising and challenging, phenomena have been explored. These include e.g. the enhanced spin- and orbital magnetism at surfaces, the discovery of new magnetic structures, the perpendicular surface magnetic anisotropy and the reorientation phase transitions, the oscillatory interlayer exchange coupling and different transport phenomena like the Giant, Tunneling and Anisotropic Magnetoresistance. All of these fields have substantial impact to technological applications, in particular, to design ultrahigh density magnetic recording media.

In this review talk, on a fairly tutorial level, I've alluded merely to some of the above topics concentrating on ground–state properties as studied by ab-initio calculations in spirit of the local spin-density approximation. A series of results on the magnetism of $3d$, $4d$ and $5d$ ultrathin films on non-magnetic substrates has been shown and discussed with special emphasis to the interrelation between magnetism and geometric structure. Different features of magnetism at surfaces and interfaces, the latter being subject to hybridization effects with the substrate, have been pointed out and compared to experimental findings. Collinear metastable states in frustrated Fe/Cu(001) thin films have been demonstrated which, in agreement with recent experiments, imply the existence of incommensurate spin-density waves as ground–state. The surface magnetic anisotropy in connection to reorientation phase transitions in thin magnetic films has been reviewed briefly on a phenomenological level. Several examples have been adduced from calculations by means of the fully–relativistic spin–polarized Screened KKR method to explore effects of the spin–orbit coupling strength, the orbital polarization, the interfacial hybridization (anomalous perpendicular anisotropy) and the layer relaxations giving rise to a reversed reorientation phase transition in thin Ni/Cu(001) films.

Electron Spectroscopy and Density-Functional Theory

A. Schindlmayr

FHI Berlin

Designed for efficient total-energy calculations, density-functional theory decouples the many-particle Schrödinger equation by mapping the interacting electron s onto a corresponding system of noninteracting electrons moving in an effective potential. As the excitation energies of these two systems differ, however, deviations between experimental spectroscopies and calculated spectra from density-functional theory are expected. The best known example is the systematic underestimation of the band gap in semiconductors and insulators. To remove these errors, the effects of exchange and correlation on individual electronic states must be properly included. They are rigorously contained in the self-energy, a nonlocal and frequency-dependent potential that describes the possible scattering processes due to the Coulomb interaction. For solids with weak or medium correlation, the so-called GW approximation for the self-energy leads to excellent agreement with experimental band structures from photoemession spectroscopy. In practice the GW approximation is evaluated perturbatively using Kohn-Sham wave functions and can hence be implemented within a density-functional context.

Magnetism Dichroism in Photoelectron Spectroscopy

C.M. Schneider

IFW Dresden

A fundamental understanding of magnetic phenomena must be based on the electronic structure of the respective materials. The appropriate technique to investigate the valence electronic states in detail is photoelectron spectroscopy. In the case of a ferromagnetic solid, an explicit or implicit spin polarization analysis of the photoelectrons is required. The implicit spin polarization analysis can be achieved by exploiting the phenomena of magnetic dichroism in the angular distribution (MDAD). This dichroism is the manifestation of the effect of optical spin orientation in ferromagnets. It requires the simultaneous influence of exchange and spin- orbit coupling. In highly symmetric geometries, the photoemission spectra can be interpreted on the basis of relativistic dipole selection rules. For perpendicularly magnetized systems probed with circularly polarized light (MCDAD), the transition matrix elements can be related directly to bulk interband transitions. For systems magnetized inplane and investigated with linearly polarized light, the transitions arise mainly due to matrix element interferences. In both cases, further details on the electronic structure can be inferred from fully relativistic photoemission calculations. The technical development of high-resolution angle-mapping photoelectron spectrometers and the availability of highly brilliant synchrotron radiation permit unparalleled investigation of the k-dependence of these effects.

Temperature dependent magnetism of solids

J. Kudrnovsky

Institute of Physics AS CR, Prague

We have determined the effective exchange interactions (EEIs) of bulk bcc-Fe and fcc-Co, Ni ferromagnets as well as magnetic overlayers Fe/Cu(001) and Co/Cu(001) covered by a Cu-cap layer of varying thickness (1-15 monolayers) in real space from first principles.

The electronic structure was determined within the tight-binding linear muffin-tin orbital method closely related to the KKR approach. We employ the so-called magnetic force theorem and construct the effective Heisenberg Hamiltonian which is then used to determine magnon dispersion laws, spin-wave stiffness constants, and Curie temperatures, the latter within both the mean-field (MFA) and random-phase (RPA) approximations. We obtain a good agreement of calculated spin-wave stiffness constants and RPA-Curie temperatures with available experimental data for the case of bulk ferromagnets.

The RPA correctly obeys the Mermin-Wagner theorem for the two-dimensional case and small relativistic effects have to be therefore considered in order to obtain a non-vanishing value of the Curie temperature. Calculations give an oscillatory Curie temperature of magnetic overlayer as a function of the cap-layer thickness in a qualitative agreement with recent experiments and its values are in better agreement with experiment as compared to the values obtained in the MFA. The origin of these oscillations can be traced down to quantum-well states formed in the Cu-cap layer sandwiched by the magnetic layer and by the vacuum which, in turn, influence properties of the magnetic layer.

In the last part we have presented new results for the electronic structure, magnetic properties, and Curie temperatures of the GaAs-based magnetic semiconductors with Mn-impurities. The special emphasis was put on the effect of As-antisites and their influence on the Curie temperature.

In collaboration with I. Turek, V. Drchal, F. Maca, J. Masek, P. Bruno, and P. Weinberger

Applications to Magnetoelectronics

P. H. Dederichs

Research Center Jülich

In this review we give a short introduction into magnetoelectronics, meaning a future powerful electronics, where both the charge as well as the spin of the electron can be manipulated by electric and external or internal magnetic fields. We then discuss the problem of spininjection, which is at present considered as a bottleneck for spindependent semiconductor devices and applications. In particular we consider the ballistic spininjection from the ferromagnet Fe into the semiconductors ZnSe and GaAs. Starting from the ground state calculation for the epitaxial Fe/ZnSe(001) and Fe/GaAs(001) systems we discuss three types of injection processes: injection of hot electrons, injection of thermal electrons and injection by a tunneling barrier. The calculation of the conductance by the Landauer formula shows, that these interfaces act like an ideal spinfilter, with spinpolarisations as high as 99 %. This can be traced back to symmetry of the Fe bandstructure along the (001) direction.

The workshop program

	TUE **19/02**	**WED** **20/02**	**THU** **21/02**	**FRI** **22/02**	**SAT** **23/02**
8^{45}		DFT	REL	DFT+SPEC	
9	Welcome	Engel	Gyorffy	Schindlmayr	
9^{15}					
9^{30}		XAS	XMO	PES	
9^{45}		Baberschke	Mertins	Schneider	
10	KKR1	(Expt.)	(Expt.)	(Expt.)	
10^{15}	Temmerman	COFFEE	COFFEE	COFFEE	
10^{30}					
10^{45}		SPEC1	SPEC2	TEMP	
11	COFFEE	Strange	Strange	Kudrnovsky	
11^{15}					
11^{30}	KKR2	CPA	MAG	SURF	access
11^{45}	Ebert	Turek	Dederichs	Szunyogh	to the
12					computer
12^{15}	FAQ/Exerc.	FAQ/Exerc.	FAQ/Exerc.	FAQ/Exerc.	system
12^{30}					possible
12^{45}					
13					
13^{15}	LUNCH	LUNCH	LUNCH	LUNCH	
13^{30}					–
13^{45}					
14					
14^{15}					some
14^{30}					tutors
14^{45}	xband	E(k)	XAS	VB-XPS	will be
15					present
15^{15}	SCF	DOS	EXAFS	CL-XPS	
15^{30}					
15^{45}					
16	COFFEE	COFFEE	COFFEE	COFFEE	
16^{15}					
16^{30}			XMO	MCP	
16^{45}	SCF	ground			
17		state	XRS	APS	
17^{15}		properties			
17^{30}	CPA		XES	AES	
17^{45}					
18				closing	

Speakers:

KKR1	W.M. Temmerman	Introduction to bandstructure calculations
KKR2	H. Ebert	The Munich KKR-package
DFT	Engel	Density functional theory for magnetic solids
XAS (Expt.)	K. Baberschke	Magnetic dichroism in X-ray absorption
SPEC1	P. Strange	Single particle description of electron spectroscopies
CPA	I. Turek	CPA alloy theory and applications
REL	B.L. Gyorffy	Relativistic effects
XMO (Expt.)	Ch. Mertins	X-Ray Magneto-Optical Polarization Spectroscopies
SPEC2	P. Strange	Calculation of electronic excitation spectra
SURF	L. Szunyogh	Surface magnetism
DFT+SPEC	A. Schindlmayr	Electron spectroscopy and density functional theory
PES (Expt.)	C. M. Schneider	Magnetic dichroism in photoelectron spectroscopy
TEMP	J. Kudrnovsky	Finite temperature magnetism
MAG	P. H. Dederichs	Applications in magneto-electronics

List of participants

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Engel, Eberhard – J.W.Goethe Universität Frankfurt, Germany
Ernst, Arthur – MPI für Mikrostrukturphysik Halle, Germany
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Schneider, C. M. – IFW Dresden, Germany
Strange, Paul – University of Keele, UK
Szotek, Z. (Dzidka) – Daresbury Laboratory, Warrington, UK
Szunyogh, Laszlo – Technical University of Budapest, Hungary
Temmerman, Walter – Daresbury Laboratory, Warrington, UK
Turek, Ilja – Academy of Sciences of the Czech Republic, Brno, CZ

3 News from New Research Training Network on f-electron Physics (RTN2)

3.1 RTN2 Postdoctoral Positions Announcement

A new EU sponsored Research Training Network will be launched on September 1, 2002, with a duration of 4 years. The Network research comprises theoretical *ab-initio* investigations of the physical properties of materials containing atoms with incompletely filled f-shells. The research has two threads: **a)** the application of existing methodology (LSD, SIC-LSD, LDA+U, Orbital Polarization etc.) to specific scientific problems of high current priority, and **b)** the development of new methodology (integration of many-body techniques into DFT based codes, Dynamical Mean Field Theory, LDA++ etc.), for a more accurate description of f-electron systems. More details can be found on

`http://www.ifa.au.dk/~svane/rtn.htm`

The Network will finance a number of **Post-doctoral Positions** at the following Network partners:

1. Århus University **DK**,
   (Axel Svane) svane@ifa.au.dk
2. Daresbury Laboratory **UK**,
   (Walter Temmerman) W.M.Temmerman@dl.ac.uk
3. Institute for Solid State and Materials Research, Dresden **D**,
   (M. Richter) M.Richter@ifw-dresden.de
4. Katholieke Universiteit Nijmegen **NL**,
   (A. Lichtenstein) A.Lichtenstein@sci.kun.nl
5. Ecole Normale Superieure, Paris **F**,
   (A. Georges) Antoine.Georges@lpt.ens.fr
6. Uppsala University **SE**
   (O. Eriksson) olle.eriksson@fysik.uu.se
7. Materials Design s.a.r.l., LeMans **F**
   (E. Wimmer) ewimmer@materialsdesign.com

If you are interested in learning more details about the Network and/or any of these positions, you are welcome to contact any of the above Network team leaders.

Axel Svane, Network Coordinator

4 News from the TMR Network ("Psi-k")

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

4.1 Fourth Annual Report of TMR-Network: "Psi-k"

Reporting period: March 1, 2001-February 28, 2002

This Network is concerned with atomic scale computer simulation methodology to understand complex properties and processes in solids and at solid surfaces. The Network is structured around 8 subprojects with 8 partners in **DK**, **FR**, **GB** (2), **DE** (2), **AT** and **FI**. During the fourth year of operation the Network has hired two more young researchers, while two have left the Network. Hence, at present, 5 young researchers are financed by the TMR grant, and a total of 66.5 man months of PostDoc training has been delivered in the past year. One more PostDoc starts March 2002, while a second will start in May 2002. Of the two PostDocs who have left, one accepted a job in computing (system administration), while the other has entered a tenure-track academic position. 10 joint papers have been published. Other principal Network activities include the organization of 3 workshops. As of September 24, the following changes were made to the Network Contract: The Network operation has been prolonged to a fifth year, finishing at the end of February 2003, and the partners MSI and TUWIEN have been exchanged with new partners: the Institut Superieur des Materiaux du Mans (ISMANS) in LeMans, **FR**, and the University of Vienna, (UNI-WIEN) **AT**, respectively. Both of these changes originated from the movements of the scientific leaders of the MSI and TUWIEN partners.

The status of the scientific subprojects is as follows:

Surfaces

This subproject, aiming at an ab-initio description of chemical reactions on iron-oxide surfaces, has been inactive for the past two years due to the move of scientist-in-charge Prof. E. Wimmer from partner MSI. With the new Network structure now in place, the subproject is revived according to the revised work plan (October 2000).

Two new network Postdocs start (one as of March 1st 2002) on this subproject, for a total of 18 Postdoc man months in the last year of Network operation. These will be based with partner ISMANS.

Surface physics remains an active area of application of the codes developed under subprojects **Magnetism** and **LAPW**, and several papers have been published.

f-electrons

The **f-electrons** subproject has a PostDoc associated with the Århus partner (L. Petit, **LU**). Applications to 5f systems continue to dominate the research. Three joint publications have appeared during the reporting period, on the electronic structure of monopnictides and monochalcogenides of Am and Pu. Papers on applications to Np and U compounds have been submitted, while several projects are ongoing, including UX binary compounds, 4f and 5f oxides, $AcRh_3$ intermetallics and improved models of fluctuating f-electrons. The strong collaboration between the Århus and Daresbury partners continues investigating both 4f and 5f systems and comparing isoelectronic 4f and 5f compounds. The study of the role of 4f elements in high T_c superconductors continues.

The implementation of full-potential total energy has been partly overtaken by events. In particular, it has become more important to speed up the SIC computer codes to tackle more complicated systems. For this we have in the last year parallellised the code, and also looked at theoretical new developments to make the formalism simpler. A simpler SIC formalism would allow the inclusion of the self-interaction corrections in other major band structure codes such as the KKR, the LAPW and FP-LMTO, thus solving the full-potential issue. Further, it could be applied to the KKR-CPA (coherent potential approximation) allowing for the first time to study *random* distributions of localised states. With external team member Karlsruhe, a perturbation theory is being developed for calculating magneto-crystalline anisotropy and anisotropy in the orbital moments in terms of the non-relativistic Green's functions. In this manner we can relate directly the measured anisotropy of orbital moments (via sum rules) to element and site specific magnetocrystalline anisotropy.

Interfaces

One Network PostDoc (A. Marmier, **FR**) is associated with the **Interfaces** subproject and based with the Belfast partner. Dr. Marmier is working on ab-initio calculations and has made valuable progress in calculating the dynamics and free energy of an oxide surface. In a first paper (to be published) he tests the quasiharmonic formalism with two different semi-empirical shell models, in order to check convergence with k-points and cell size on system sizes too large for ab initio calculation. The gratifying discovery is that surface free energy can be calculated accurately with a coarse (2-point) k-point mesh, which enabled the ab initio calculations of it with frozen phonons in supercells of only 60 atoms. These ab initio calculations are reported in a second paper (in preparation). The decrease in free energy with temperature is similar with all the models tested. The quasiharmonic approximation proved to work up to about 900K, but broke down thereafter. Dr. Marmier also showed that anharmonicity would not account for the discrepancies between ab initio surface relaxations and experimentally determined ones. This makes the alternative explanation of surface impurities more likely, but so far the experimentalists have failed to detect any. In Stuttgart, work has started on calculations for transition metals on $SrTiO_3$.

Magnetism

A new Network Postdoc, Dr. Martijn Marsman **NL**, started with partner UNI-WIEN. He continues the application of the developed noncollinear magnetism code to several magnetic systems. All milestones of this subproject have been reached, with the exception of the spin-dynamics, which will, however, happen in the near future.

One of the main goals of the project is the implementation of a noncollinear magnetic moment capability in the major electronic structure codes: VASP, FLEUR, LMTO etc. This taks was essentially completed already during the last year. As an additional feature a capability to treat incommensurate spin-helices using the generalized Bloch-theorem of C. Herring has been implemented in VASP. This new capability has been used to investigate the stability of spin-helices in γ-Fe and the correlation between shear-distortions on magnetic ordering.

The investigations of noncollinear magnetism in the complex polymorphic phases of Mn have been continued to the β-Mn phase. This completes the investigation of phase stability of Mn so that a complete picture of the structural and magnetic phase diagram of this most complex of all metallic elements is now available. The investigations of Mn-based compounds have been extended to the Laves-phase YMn_2 and to Y-Mn-Sn phases with frustrated magnetic interactions in triangular or Kagomé-layers. Work on noncollinear magnetism in ordered and partially disordered manganite compounds showing giant or colossal magnetoresistance have been continued. Canted magnetic structures could be identified in partially disordered $La(Ca_xSr_{1-x})MnO_3$ compounds. A new project concerns the exotic electronic and magnetic properties of $FeAl_2$. This compound crystallizes in a complex triclinic structure and has been reported to show spin-glass behaviour at low temperature.

The possibility of the formation of spin-waves in ultrathin Fe films epitaxially grown on Cu(100) (as recently proposed by Kirschners group in Halle) has been investigated. It could be shown that in ultrathin films, spin-wave formation is suppressed by strong surface- and interface effects. On the other hand, the long-period reconstructions observed by STM in Fe/Cu(100) films of various thicknesses could be explained in relation to the structural and magnetic properties of bulk γ-Fe. Investigations of commensurate antiferromagnetism versus spin-density waves for bulk Cr, ultrathin Cr/Fe(100) films and Cr/Fe multilayers have been performed.

LAPW

In the reporting period, no Network PostDocs have been associated with the LAPW subproject. All of the subtasks of this project have been accomplished.

The LAPW research activity has focussed, as planned, on the continued application of the FLAPW codes to the investigation of growth and the dynamics of catalytic reactions by the external team member of the surface node at FHI in Berlin, as well as to the investigation of magnetic systems by the Jü lich partner in collaboration with the external team member Uppsala. The latter was mostly on spin-orbit related questions of nano-wires and of the magneto-structural stability of fcc-Fe.

Two major turns in physics, which were not apparent as the proposal was written four years ago, are the rapidly increasing importance of the transport properties of nanoelectronic structures and of organic materials. Since in organic materials the electron-phonon interaction is very important an additional effort has been undertaken to develop the linear-response theory and the ballistic transport properties within the FLAPW method. These development were made in the WIEN99 and the FLEUR codes. The implementation of the linear-response theory provides a framework in which the electron-phonon matrix elements can be calculated using all electrons and is therefore applicable also to perovskites and magnetic systems, which are very difficult to treat with the pseudopotential method. The work is a collaboration of the Graz and Uppsala groups.

The FLAPW method has been extended to a Green function FLAPW method to calculate the transfer matrix. This allows the calculation of scattering states and the complex band structure, and opens the perspective to calculate transport properties with the FLAPW method in the future. A paper is accepted for publication in Phys. Rev. B.

Excitations

Two Network PostDocs have been associated with the **Excitations** subproject in the reporting period, (J. J. Hogan-O'Neill, **UK**, until July 2001, and from August 2001, M. P. Jigato, **E**, both based with the Helsinki partner). Dr. Jigato is guaranteed to stay in Helsinki until the end of 2003, his salary being paid by other sources after the end of the present Network.

The research comprises the implementation of novel schemes to account for excitations beyond the standard LDA, or GGA, description.

Dr. Hogan-O'Neill completed a study of a quantum dot coupled to d-wave superconducting leads. This project, which has been carried out in collaboration with the external team member at Chalmers University of Technology, has been presented as a short talk at the American Physical Society March Meeting (Seattle, USA, March 2001). An article about the work is being finalised.

The main activity at present is the implementation of time-dependent density functional theory (TDDFT) within the real-space code (MIKA) developed at Helsinki. We have collaborated intensively with the group of Prof. Angel Rubio at Donostia International Physics Center, San Sebastian, Spain. The advantage of using a real-space, real-time approach in TDDFT is the access to the full response (nonlinear excitations) of the system with a much simpler computational implementation.

The applications under study at present include the ground states and photoabsorption spectra of quantum dots, carbon-based fullerene structures, and semiconductor (Ge) clusters.

Dr. Perez Jigato has visited the group at San Sebastian in January 2002, and has interacted with the network partner in Wü rzburg.

Superconductivity

Two Network PostDocs are associated with the **Superconductivity** subproject, (L. Fast, **SE** until October 2001, and N. Lathiotakis, **GR**, both based with the Wü rzburg partner).

The work on density functional theory for the superconducting phase was continued. First results on the transition temperatures of conventional superconductors have been published. So far, attemps to solve the nonlinear gap equation (to determine the gap at zero temperature, the critical magnetic field, etc.) were not successful. Work on improved functionals as well as refinements of the computer codes to solve the gap equation are ongoing. In particular, The LDA-type functional first suggested by Kurth et al., was further developed and investigated. It was found that this functional, when applied to the uniform gas, does indeed yield a superconducting ground state for sufficiently large r_s and sufficiently high angular momentum (similar to the Luttinger-Kohn mechanism). These results are currently being prepared for publication.

A review article on relativistic effects in superconductors was published. The anomalous spin-orbit term appearing in this theory is now being implemented to investigate the dichroic response of normal-superconducting-normal multilayers (where its influence is expected to be particularly large).

The collaboration between partners Wü rzburg and Daresbury and the Bristol group continued, completing a review article on semi-phenomenological models for High Tc superconductors. A new project, aimed at a study of the Ruthenocuprate ($\mathrm{RuSr_2GdCu_2O_8}$) was formulated. This is a fascinating material as it is host to coexistence of ferromagnetism (with a transition temperature T_m = 132 K) and superconductivity (with T_s = 40 K). The developed methodology is suitable for generating a spin polarized, first-principles, down-folded, tight-binding model with a phenomenological electron-electron interaction constant operating in the CuO plane. It is assumed that the Ru layers are ferromagnetic and the superconductivity, in the exchange field, mainly confined to to the CuO plains. In this configuration the ground state is expected to be of the Fulde-Ferrel-Larkin-Ovchinnikov type. The theory and the corresponding computer codes have been generalized to deal with this very interesting case and first calculations are in progress.

Training and Dissemination

This subproject is concerned with training and dissemination. This encompasses the publication of the Psi-k Newsletter every two months and organisation of topical workshops and hands-on courses to train young researchers in the methodology of electronic structure calculations for materials properties, including practical training in the application of computer codes. The Daresbury partner coordinates these activities, which involve all Network partners.

A workshop on 'Non-collinear Magnetism,' was organised in Wien, in March 2001, with 35 attendees. A workshop on 'The physics of f-electron systems' was organised in Daresbury in April 2001, with 37 attendees. The hands-on course: 'Full-Potential APW+lo Calculations with the new WIEN2k Code', Wien, September 2001, was co-sponsored by the Network. Full reports on these three events can be found in the Psi-k Newsletters (no. 44, and 45). Together with the Stuttgart node, the Belfast node organised and chaired a joint Psik-CECAM workshop on oxide-metal interfaces which took place place in Lyon, 4-6 October. Representatives from the microelectronics, automobile and paint industries contributed talks, together with experimentalists and representatives from our theoretical network.

During the reporting period, six Newsletters were published, in April, June, August, October, December 2001 and February 2002. This Newsletter is e-mailed to more than 900 e-mail addresses and is also available on the home page of the TMR Network. The Majordomo mailing lists and the psi-k www pages are kept up-to-date by this subproject.

The fifth Network Management Board Meeting took place in Paris on October 6, 2001.

Axel Svane, Network Coordinator

5 News from the ESF Programme

"Towards Atomistic Materials Design" (Psi-k)

5.1 Call for Workshop Proposals for 2003

It is time to consider proposals for workshops to be held in 2003 for (partial) funding by the ESF Psi-k Programme. The new Psi-k proposal has been selected by the European Science Foundation in April, but now awaits actual funding by the individual national research councils.

Proposals should be submitted by email (in the form of a single simple email letter WITHOUT ATTACHMENTS OR LATEX, just plain ascii) to the Psi-k Programme secretary, Walter Temmerman, at

psik-coord@dl.ac.uk

by August 31, 2002, and should include the following points (preferably numbered in this order).

1. Title and purpose of the workshop, with names and addresses (including email) of the organisers.
2. The scientific content and why a workshop would be useful at this time.
3. A tentative list of speakers whom it is hoped to have.
4. The number of participants it is planned to invite or attract, and their scientific involvement, eg. as simulators, related experimentalists, code developers etc., and young scientists in the subject.
5. Plans for a tutorial element and for attracting new researchers into the subject of the workshop. (If this is thought inappropriate for this workshop, please discuss why.) The purpose of the ESF Psi-k Programme is
6. A budget, expressed in Euro, and how much is being applied for from the ESF Psi-k Programme. This support in the past has been limited to ∼9k Euro.
7. A statement of other organisations which will be applied to for co-sponsorship and additional funding, eg. the RTN Network on Computational Electronics, other RTN Networks, CECAM, CCP-9 in the UK, etc..
8. Where it is hoped the Workshop would be held. (Joint workshops with CECAM are normally held at CECAM in Lyon.)
9. Very little money is available for American participants. If there is a wish to have several, I suggest to include an American co-organiser with an NSF grant, who can perhaps/probably get a few thousand dollars extra for this purpose from the NSF International Materials Science Program (director Lance Howarth).

Volker Heine
Chairman of ESF Psi-k Programme
e-mail: vh200@phy.cam.ac.uk

5.2 Join a Working Group in the new ESF Psi-k Programme

This is to inform everyone about the present situation regarding our proposal to the European Science Foundation (ESF) for a new 5-year Psi-k Programme. One of its main features is a set of 15 Working Groups covering various areas of research, and anyone in Europe can participate in those.

First the present situation:- Our proposal has now been selected for support by the ESF, but the actual money has to come from the individual national research councils of the European countries (more or less all Europe, not just the EU). They will get asked from early June whether they want to join our Programme, and we hope they will! If you have any influence in the required places, please use it! Also please let your national Psi-k representative know: the name can be found from the planned steering committee listed in our proposal which you can find on the website **http://psi-k.dl.ac.uk/proposal**.
Incidentally, we got 5 very supportive referee reports: they could not have been nicer. I think this is a great tribute to the very collaborative way our research community works.

The proposal may be seen on the website, both in a preliminary 6-page version and in a final 15-page version.

Its main new feature is a set of 15 WORKING GROUPS covering some major areas of research, but of course not all areas. Have a look at them on the website, which contains a page or so of write-up on each one. If you would like to participate in one (or perhaps more) of these, then please get in touch with the Spokesperson for the Working Group whose email is also given on the website by the description of the Group. Then bring along your suggestions for particular collaborations. Remember, Psi-k is a 'bottoms-up' organisation. The activities of Psi-k are the activities of those who participate. There is no 'membership'. Every researcher in our field of ab initio simulation can automatically participate, even scientists from countries who do not pay (as long as there are not too many of you!). Of course workshops etc. can be proposed in areas other than the 15 Working Groups.

Other activities of Psi-k will carry forward: workshops, training including hands-on tutorials, the Psi-k Newsletter, individual visits that are difficult to fund in other ways, a big conference again in 2005, contact with industry which I hope can be increased, and collaboration with other conferences and organisations to show the contribution of our subject.

An idea that has just come up is that perhaps we can be recognised by the European Commission as a 'European infrastructure' under the new 6th Framework. It should give Psi-k a longer term existence, because we cannot apply again to the ESF five years from now: we are already anomalous in having a second Programme.

Peter Dederichs will be the chairman of the new Psi-k from the time when he retires in March 2004, and I will continue until then.

Volker Heine
Cambridge, May 16, 2002

5.3 Reports on Collaborative Visits

Report on a collaborative visit of Diemo Ködderitzsch (Martin-Luther-Universität Halle-Wittenberg, Germany) to Professor Walter Temmerman's group (Daresbury Laboratory, UK)

April 4-6 and 12-25, 2002

Within the STRUC-Ψ_k ESF Programme, I spent over two weeks (4-6.04.2002 and 12-25.04.2002) at Daresbury Laboratory, in the group of Professor Walter Temmerman continuing our collaboration on the electronic structure of surfaces and interfaces of strongly correlated transition-metal oxides.

During my stay we concentrated on two main tasks.

1. One aspect of my PhD project is a description of the magnetic interactions in the strongly correlated transition-metal oxides. A paper on the magnetic interactions at the NiO (100) surface and their relation to bulk NiO was finalised and submitted during my stay at Daresbury Laboratory.

2. Single crystal oxide barriers appear to be candidates for TMR junctions. Electronic structure calculations for the system Fe/MgO predicted a high magnetoresistance (Butler *et al.* PR**B** **63**, 054416 (2001)). These calculations were performed in the framework of LDA. As there is however oxygen incorporated into the Fe/MgO interface (Meyerheim *et al.* PRL **87**, 076102 (2001)), resulting in a single FeO layer, strong correlations might occur, having a significant impact on the electronic structure of this interface. During my stay at Daresbury Laboratory we discussed and investigated the use of the self-interaction corrected LSD (SIC-LSD) (A. Svane, O. Gunnarsson, PRL **65**,1148 (1990); Z. Szotek *et al.*, PR**B** **47**, 4029 (1993)) to explore the importance of including these effects in calculations. We performed preliminary electronic structure calculations for that system using the Daresbury SIC-LSD code. The Fe/MgO interface was modelled using a super-cell approach, sandwiching MgO between layers of iron. In accord with the structural data mentioned in the paper above, oxygen was incorporated into the interface.

   We started with the standard LSD calculations to test the sensitivity of results depending on the choice of such parameters as the number of Fe or MgO layers and displacement of the interface oxygen atom in the direction perpendicular to the interface. We observed a strong dependence of the results on the oxygen displacement. Then, we considered the self-interaction correction of $3d-$electrons on the Fe sites in the single FeO layer at the interface. We found out that correcting five majority and no minority electrons was favoured over the choices where the sixth d electron was localised in any of the orbitals of the d minority manifold, leaving Fe in the FeO layer in a trivalent state (Fe^{3+}). This choice of SI-corrected states also led to a total energy which was lower than that of the LSD solution. Therefore, we concluded that the inclusion of SIC for the Fe d electrons at the interface was of importance for the electronic structure and would have an impact on transport properties.

To summarise, during my stay at Daresbury Laboratory we finished a collaborative paper on the subject of magnetic interactions at the NiO (100) surface and started a project on the electronic structure of the Fe/MgO interface.

I am grateful to the Psi-k network for its support.

Diemo Ködderitzsch
Halle, April 30.

5.4 Report by the Psi-k 'consultant' on the first CECAM Advisory Committee on 6 April, 2002

This committee is a new development to help the CECAM director keep in touch with the broad range of researchers doing atomistic computer simulation of condensed matter. The first two 'consultants' attended, namely Professor Mike Klein (Univ. of Pennsylvania) and myself, in addition to the CECAM director, Professor Michel Mareschal. It is envisaged that two more consultants will be appointed by the next director who will be selected soon. Professor Giovanni Ciccotti also attended by invitation. (He was the first director to start rebuilding CECAM after the debacle of the 1980s. Directors are now appointed for 4 years.)

The discussion included the following areas.

1. The present situation at CECAM and the role of the Advisory Committee
2. Review of CECAM's 2002 programme
3. Ideas for workshops and tutorials in 2003
4. 'Network of Excellence' on simulation of soft condensed matter
5. Future development of CECAM

Under item 3, it was felt desirable for a few workshops and tutorials to be stimulated by the director on subjects considered to be particularly relevant, of course in addition to proposals received in response to the open call.

Under item 4, Mareschal reported plans to apply for an EU 'Network of Excellence' on simulation of soft condensed matter, based on CECAM and the ESF SIMU Programme, including some ab initio simulation. (Parrinello is a member of SIMU.) I said he was welcome to draw in the people from our Working Group 12 on applications to biology.

Under item 5, Mareschal reported on his discussion with the European Commission who said that 'human' infrastructures such as CECAM and the Psi-k movement are not ruled out for consideration as infrastructures under the Sixth Framework. I will report on this further to the Psi-k committee.

Volker Heine
Cambridge, 29 April, 2002

5.5 Reports on ESF Workshops

5.5.1 Report on Mini-2002 Workshop

"Total Energy Methods in Computational Condensed Matter"

Sponsored by
European Science Foundation Programme "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" (Psi-k)
Gobierno de Canarias, Ministerio de Ciencia y Tecnología (SPAIN)
Universidad de La Laguna (ULL) and Universidad del Pais Vasco (UPV/EHU)

The Workshop was held in the Facultad de Fisica of the Univerisdad de La Laguna from 10th to 12th January 2002.

It was organised by **Alfonso Muñoz**, Universidad de La Laguna, Tenerife, Spain
Andres Mujica, Universidad de La Laguna, Tenerife, Spain
Angel Rubio, Universidad del País Vasco, San Sebastián, Spain

Scientific Committee

A. Baldereschi (EPFL, Laussanne, Switzerland)
S. Baroni (SISSA, Trieste, Italy)
M. Gillan (University College of London, London, UK)
K. Kunc (CNRS, University P. and M. Curie, Paris, France)
S.G. Louie (University of California - Berkeley, USA)
R. M. Martin (University of Illinois at Urbana-Champaign, USA)
M. Methfessel(Institut fur Semiconductor Physics, Frankfurt-Oder, Germany)
R.J. Needs(Cambridge University, Cambridge, UK)
P. Ordejon (ICMAB-CSIC, Barcelona, Spain)
M. Parrinello (Max Planck Institut fur Festkorperforchung, Stuttgart, Germany)
K. Terakura (NAIR, Tsukuba, Japan)
D. Vanderbilt (Rutgers University, New Jersey, USA)
E. Wimmer (Materials Design, Le Mans, France)

The Workshop was devoted to recent advances in computational condensed matter physics, based on realistic calculations of the electronic structure of polyatomic systems. It was concerned with *ab initio* calculations of structural and electronic properties of a wide class of systems in condensed matter as well as atomic and molecular physics (nanostructured materials) and biophysics. New advances in computational techniques for structural and response calculations were presented. The aim of this workshop was to bring together researchers of different backgrounds (density functional, many-body, and nuclear physics approaches) in order to assess the present status of the *ab-initio* computation of, and to make connection with, up-to-date experimental characterization techniques. There were 22 invited speakers and a full poster session. Discussions were lively and not restricted to a limited group of people.

The program and the discussions have been centered around several main questions:

- Density-functional molecular dynamics and thermodynamical properties; Phase transitions;
- Large-scale electronic structure calculations; Linear-scaling methods;
- Many-body total-energy techniques for real materials;
- Dynamical mean-field theory and connection to classical DFT methods
- Combination of DFT and empirical tight-binding
- Chemical reactions in condensed phases;
- Electron dynamics and excited states; Time-dependent density functional theory
- Applications to Biophysics
- Surfaces and other low-dimensional systems; nanoscience

In fact, the workshop has shown to continue an important tendency which has grown out of the previous workshops of this series started in Oxford (1983) and continued in Braunschweig (1984) and in Trieste (1987, 1989, 1991, 1993, 1995, 1997 and 1999).

It has also been very important that a big number of spanish and EC PhD students and post docs could participate, thanks to the financial support of ESF/Psi-k. After the workshop, on 14-15 January, a Tutorial total energy pseudopotential plane waves method was developed with the participation of 14 students. The Tutorial included a morning session (3 hours) on Monday 14, with lessons concerning the theoretical basis and 3 practical sessions (11 hours) with applications.

TENERIFE 2002. CONFERENCE PROGRAM

THURSDAY, JANUARY 10

09:00-09:10 **Opening Remarks**

INVITED SPEAKERS

Nanostructures and Interfases Session. Chairman: D. VANDERBILT

9:10-10:00 **Risto M. Nieminen** (*Helsinki University of Technology, Finland*)
"Quantum dots in magnetic field - current-DFT calculations in real space"

10:00-10:50 **Carla Molteni** (*Cavendish Laboratory, University of Cambridge, UK*)
"Nanostructures under pressure"

10:50-11:15 COFFEE-BREAK

11:15-12:05 **Luciano Colombo** (*Universitá degli Studi di Cagliari, Italy*)
"Structural and electronic properties of a-Si/c-Si interface"

12:05-12:55 **Richard J. Needs** (*Cavendish Lab., University of Cambridge, UK*)
"Structural relaxation in electronically excited poly(para-phenylene)"

13:00-14:30 LUNCH

Many-Body Approaches Session. Chairman: K. KUNC

14:30-15:20 **Ferdi Aryasetiawan** (*Res. Inst. for Comput.l Sci., Tsukuba, Japan*)
"Total energy method from many-body formulation"

15:20-16:10 **A. Georges** (*Ecole Normale, France*)
"Recent advances in the dynamical mean-field theory of strongly correlated electron systems"

16:10-16:30 COFFEE-BREAK

16:30-17:20 **Francesc Illas** (*Universitat de Barcelona, Spain*)
"Ab initio study of magnetic interactions and determination of effective Hamiltonian parameters in High Tc superconductors"

17:20-18:10 **E. Koch** (*Max Planck Institute, Sttutgart, Germany*)
"Physics of the superconducting Fullerenes"

18:10-20:00 **POSTER SESSION and GET TOGETHER PARTY**

P. Palacios et al. (*Univ. Politecnica de Madrid, Spain*)
"Theoretical phonon studies of semiconductor structures"

D. Vanderbilt et al. (*Rutgers university, USA*) "A k-space approach to finite electric fields in insulators"

Magali Benoit et al. (*Universite Montpellier II, France*)
"Structural properties of glassy and liquid sodium tetrasilicate: comparison between ab initio and classical molecular dynamics simulations"

M. Profeta et al. (*Universite Pierre et Marie Curie, Paris VI, France*)
"Theory of resonant Raman scattering of tetrahedral amorphous carbon: Ab-initio calculation of 170 NMR spectra in oxides"

P. Garcia-Hernández et al. (*Universidad de Cantabria, Spain*)
"Silver atoms embedded in ionic lattices"

E. V. Chulkov et al. (*Universidad del Pais Vasco, Spain*)
"The lifetimesof quasi-particle excitations in para- and ferromagnetic transition metals: LMTO GW approach and scattering theory model calculations"

Jeil Jung et al. (Univ. Nacioanl de Educacion a Distancia, Spain)
"Two interacting electrons confined in a sphere: some exact and DFT results"

J. Junquera et al. (*Universite de Liege, Belgium*)
"Structural and electronic properties of nanosized ferroelectric hybrid structures"

Y. Al-Douri (*Univ. of Sidi Bel-Abbes, Algeria*)
"The pressure effect on the electronic properties of III-V compounds by semi-empirical tight-binding method"

Jose Gabriel Díaz et al. (Univ, Jaume I, Castellon, Spain)
"Multilayer nanocrystal in a magnetic field"

20:45-22:00 **Visit to the old part of San Cristóbal de La Laguna**

FRIDAY, JANUARY 11

Chemical and Biology Session. Chairman: R.J. NEEDS

09:00-09:50 **Nicola Marzari** (*MIT, USA*)
"Real-time chemical reactions via ab-initio molecular dynamics"

09:50-10:40 **Nicolas Lorente** (*Lab. Collisions., Université Paul Sabatier, France*)
"Study of molecule chemisorption on noble metal surfaces"

10:40-11:10 COFFEE-BREAK

11:10-12:00 **D. Alfe'** (*University College London, UK*)
"Complementary approaches to the ab-initio calculation of melting properties"

12:00-12:50 **Carme Rovira** (*Universitat de Barcelona, Spain*)
"First principles simulations of ligand binding to hemeproteins"

13:00-14:30 LUNCH

Excitations and TDDFT Session. Chairman: R.M. MARTIN

14:30-15:20 **Pedro M. Echenique** (*Universidad del Pais Vasco, Spain*)
"Lifetime of electrons at surfaces"

15:20-16:10 **Lucia Reining** (*Ecole Polytechnique, France*)
"Effects of long-range interactions in the absorption and loss spectra of finite and infinite systems"

16:10-16:30 COFFEE-BREAK

16:30-17:20 **F. Mauri** (*Universite Paris VI, France*)
"All-electron magnetic response with pseudopotentials: EPR g-tensor of defects in solids and NMR chemical shifts"

17:20-18:10 **E. V. Chulkov** (*Universidad del Pais Vasco, Spain*)
"Quasiparticle dynamics at bulk metals and at interfases"

20:15 CONFERENCE DINNER

SATURDAY, JANUARY 12

Methods Session. Chairman P. ORDEJON

09:00-09:50 **Rubén Pérez** (*UAM, Madrid, Spain*)
"Exchange-correlation Energy as a function of the orbital occupancies: Implementation on First-Principles Local Orbital Method"

09:50-10:40 **J. Gale** (*Imperial College, UK*)
"Towards large-scale electronic structure calculations with parallel SIESTA"

10:40-11:00 COFFEE-BREAK

11:00-11:50 **Mads Brandbyge** (*Tech. Univ. of Denmark, Denmark*)
"Density functional method for nonequilibrium electron transport"

ORAL CONTRIBUTIONS

11:50-12:15 **Silvana Botti** (*Ecole Polytechnique, France*)
"Ab initio calculations of the static dielectric tensor of GaAs/AlAs superlattices"

12:15-12:40 **Mariví Fernandez-Serra** (*Depart. of Earth Sci., U. Cambridge, U.K.*)
"Hessian model for acelerating ab-initio geometry optimizations"

12:40-13:00 **R.M. Martin: CONCLUDING REMARKS and CONFERENCE CLOSING**

13:00-14:30 LUNCH

14:45 CONFERENCE EXCURSION (Teide National Park)

Abstracts of Talks

Complementary approach to the ab-initio calculation of melting properties

Dario Alfe'

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University College London, Gower Street, London WC1E 6BT, U.K.

Several research groups have recently reported *ab initio* calculations of the melting properties of metals based on density functional theory, but there have been unexpectedly large disagreements between results obtained by different approaches. We analyze the relations between the two main approaches, based on calculation of the free energies of solid and liquid and on direct simulation of the two coexisting phases. Although both approaches rely on the use of classical reference systems consisting of parameterized empirical interaction models, we point out that in the free energy approach the final results are independent of the reference system, whereas in the current form of the coexistence approach they depend on it. We present a scheme for correcting the predictions of the coexistence approach for differences between the reference and *ab initio* systems. To illustrate the practical operation of the scheme, we present calculations of the high-pressure melting properties of iron using the corrected coexistence approach, which agree closely with earlier results from the free energy approach. A quantitative assessment is also given of finite-size errors, which we show can be reduced to a negligible size.

First principles calculations of ligand binding in hemeproteins

Carme Rovira

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The structural and vibrational properties of the Fe-CO bond in carbonmonoxy myoglobin (MbCO) will be investigated by means of hybrid QM/MM calculations based on density functional theory combined with a classical force field.[1] It will be shown that the Fe-CO structure is not influenced by the distal pocket conformation. In contrast, both the CO stretch frequency and the energy of the interaction between the CO and the distal histidine aminoacid (His64) depend on the orientation and tautomerization state of His64.[2] Our calculations exclude the protonation of His64 at N_δ and help the assignation of the different CO absorptions observed in the IR spectra of MbCO.[3] Further aspects of the binding of ligands in other hemeproteins will also be discussed.

[1] M. Eichinger, P. Tavan, J. Hutter and M. Parrinello. J. Chem. Phys. 110, 10452 (1999).

[2] C. Rovira and M. Parrinello. Biophys. J. 81, 435 (2001).

[3] G. U. Nienhaus and R. D. Young. Protein Dynamics. In Encyclopedia of Applied Physics, Vol. 15 G. Ed. L. Trigg. VCH Publishers, NY (1996).

Quasiparticle dynamics in bulk metals and at interfaces

E.V. Chulkov[1,2]

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[2]*Donostia International Physics Center (DIPC), 20018, San Sebastián/Donostia, Basque Country, Spain*

Screening and lifetimes of quasiparticles (electrons and holes) in bulk materials and at interfaces are of paramount importance for the description of many phenomena in condensed matter science. In this contribution we report the first-principles study of screening in simple, noble, and transition metals. We present the pseudopotential- and LMTO-GW calculation results for hole and electron lifetimes in these metals. The imaginary part of the self-energy operator as a measure of quasiparticle lifetime is calculated by using the GW approximation. We demonstrate that in general the lifetime as a function of momenta and energy shows very anisotropic behavior while for some materials like aluminium and noble metals the excited electron lifetimes may be well approximated by quadratic function. We also discuss the feasibility of the density-of-states convolution model of the scattering theory for calculations of quasiparticle lifetimes. In contrast to 3-dimensional (3D) metals the interfaces represent a typical 2D system with very different quasiparticle dynamics. We discuss this dynamics for the particular case of one monolayer of sodium on Cu(111). We show that the specific dynamics at interfaces is due to two factors: intraband transitions within the interface state band generated by the interface itself and specific behavior of the imaginary part of the screened Coulomb interaction at the interface.

Structural and electronic properties of a-Si/C-Si interface

Luciano Colombo

INFM and department of Physics, University of Cagliari (I)

Maria Peressi

INFM and Department of Theoretical Physics, University of Trieste (I)

Stefano de Gironcoli

INFM and SISSA, Trieste (I)

By combining model-potential and tight-binding molecular dynamics simulations, and ab initio density-functional-theory calculations, we investigated the mechanism governing the electronic band alignment at amorphous/crystalline silicon interfaces.

We have found that:

- The band alignment is almost vanishing for those samples where no coordination defects are present; it is however sizeable for defect-rich samples.
- The band alignment is independent of interface details for defect-free interfaces.
- The band alignment in defect-rich samples does not depend on the actual defect concentration and distribution. This behavior is ascribed to the semimetal character of the amorphous region.
- The band alignment is classified in any case as a bulk effect, mainly due to the broadening of the valence band.

A full report of this work has been published as:

M. Peressi, L. Colombo, and S. de Gironcoli, Phys. Rev. B 64, 193303 (2001).

We acknowledge computational support by INFM under the "Parallel computing initiative".

Lifetimes of electrons and holes at surfaces

P.M. Echenique[1,2]

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Surface screening and lifetimes of electrons and holes at metal surfaces are of fundamental interest in surface science: they govern the dynamics of charge and energy transfer, enter the description of such important phenomena as screening in an electrón gas, electrón-phonon coupling,

localization, quantum interference. We report first-principles and model potential calculation results for surface screening and lifetimes for holes in surface states and electrons in surface and image ptential states on clean metal surfaces. We also discuss the dynamics of excited electrons in transient states of single adatoms on Cu(100) and Cu(111). The calculations are performed within the GW approximation to evaluate the quasiparticle self-energy.

Total Energy Method from Many-Body Formulation

F. Aryasetiawan[a], T. Miyake[b], T. Kotani[c], M. van Schilfgaarde[d] and K. Terakura[a]

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[b]*Department of Physics, Tokyo Institute of Technology*
2-12-1 Oh-okayama, Meguro-ku, Tokyo 152-8551, Japan
[c]*Osaka University, 1-1 Machikane-yama, Toyonaka 560, Japan*
[d]*Sandia National Laboratory, Livermore, CA U.S.A.*

The fruitfulness of traditional many-body Green's function theory for calculating the total energy of real systems is demonstrated using the Luttinger-Ward formulation. As an application to a real system, the total energy of H_2 is calculated as a function of nuclear separation within the random phase approximation and compared with the configuration interaction and the local density approximation results. While the local density result is in large error for large separations, the present approach gives satisfactory agreement with the configuration interaction results. The method has also been applied to calculate the equilibrium lattice constants of solid Si, Na, and Cu. The role of electron correlations in the mechanical properties is discussed. The method is promising as an alternative to the quantum Monte Carlo technique.

Ab initio study of magnetic interactions and determination of effective hamiltonian parameters in High Tc superconductors

F. Illas[1], I. de P. R. Moreira[1], D. Muñand M. A. Garcia-Bach[2]

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[2] *Departament de Física Fonamental & Centre especial de Recerca en Química Teòrica, Universitat de Barcelona & Parc Científic de Barcelona, Martíi Franquès 1, E-08028 Barcelona, Catalunya, Spain*

The magnetic coupling constant of selected cuprate superconductor parent compounds has been determined by means of embedded cluster model and periodic calculations both carried out at the same level of theory. The agreement between both approaches validates the cluster model which is subsequently employed in state-of-the-art configuration interaction calculations aimed to obtain accurate values of the magnetic coupling constant and hopping integral for a series of superconducting cuprates. Likewise, a systematic study of the performance of different ab initio explicitly correlated wave function methods and of several density functional approaches

is discussed. The accurate determination of the parameters of the t-J Hamiltonian has several consequences. First, it suggests that the appearance of high-Tc superconductivity in existing monolayered cuprates occurs within J/t in the 0.20 - 0.35 regime. Second, $J/t = 0.20$ is predicted to be the threshold for the existence of superconductivity and, third, a simple and accurate relationship between the critical temperatures at optimum doping and these parameters is found. However, this quantitative electronic structure versus Tc relationship is only found when both J and t are obtained at the most accurate level of theory.

Real-time chemical reactions via *ab-initio* molecular dynamics

Nicola Marzari[1] and Roberto Car[2]

[1]*Department of Materials Science and Engineering, MIT, Cambridge MA*
[2]*Department of Chemistry and PMI, Princeton University, Princeton NJ*

The extension of the first-principles molecular-dynamics approach of Car and Parrinello (CP) to include simultaneous "on-the-fly" evolution of occupied and unoccupied electronic states is presented. The CP scheme is reformulated in the context of finite-temperature ensemble density-functional theory (eDFT) [1], adding as dynamical variables - besides the electronic wave functions - their occupation numbers and the unitary rotations among all states considered. The resulting equations of motion allow for an entire subspace spanned by states with different fractional occupations to follow adiabatically the nuclear trajectories, allowing to treat systems where e.g. the total spin changes along a reaction pathway, the total number of electrons fluctuates in grand-canonical equilibrium, or where the electrons have a finite-temperature distribution. The technique is applied to the test case of an oxygen molecule dissociating on a nanotube vacancy, using Γ-point sampling. Extensive Born-Oppenheimer eDFT simulations are used to study chemical reactions on metal surfaces (using Baldereschi-point sampling); namely, the dissociative chemisorption of chlorine on aluminum and the partial oxidation of methane on platinum. In both cases, and in spite of limited statistics, we gather fundamental and detailed microscopic information on the reaction mechanisms, the transfer of charge, and the effects of translational and vibrational energy on the dissociation dynamics.

[1] N. Marzari, D. Vanderbilt, and M. C. Payne, *Phys. Rev. Lett.* **79**, 1337 (1997).

Density functional method for non-equilibrium electron transport

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We have recently developed a first principles method [1] for calculating the electronic structure, electronic transport, and forces acting on the atoms, for atomic scale systems connected to semi-infinite electrodes with an applied voltage bias. Our method is based on the density functional theory as implemented in the well tested SIESTA package [2]. With our code, dubbed TranSIESTA, we fully deal with the atomistic structure of the whole system, treating both the contact and the electrodes on the same footing. The electron density at finite bias is calculated using non-equilibrium Greens functions (iterated until self-consistency).

In this talk we present our method and concentrate on our results for the non-linear transport of single atom wide contacts. We consider contact systems of gold and platinum connecting perfect bulk electrodes in the (111) or (100) directions. We furthermore calculate the forces acting on the contact atoms due to the non-equilibrium situation in the electronic subsystem, i.e. in the presence of an electronic current. As an example of the use of our method in molecular electronics we present results for rectification in organic single molecules.

[1] Our implementation is called TranSIESTA and is described in M. Brandbyge, J. Taylor, K. Stokbro, J-L. Mozos, and P. Ordejon, cond-mat/0110650

[2] D. Sanchez-Portal, P. Ordejon, E. Artacho and J. Soler, Int. J. Quantum Chem. 65, 453 (1997)

Quantum dots in magnetic field - current-spin-DFT calculations in real space

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The electronic structures and total energies of circularly confined two-dimensional quantum dots and quantum-dot dimers in finite magnetic fields are investigated using the current-spin-density-functional theory (CSDFT). The relevant differential equations are solved using the recently developed, symmetry-unrestricted real-space algorithm which effectively utilizes multigrid acceleration schemes. In particular, I discuss in this talk the results obtained for a six-electron dot as a function of confinement and magnetic field, and those for a quantum-dot dimer as function of separation. The results are compared against Quantum Monte Carlo simulations for the same structures. The role of symmetry-breaking solutions obtained from the CSDFT calculations is discussed.

Effects of long-range interactions in the absorption and loss spectra of finite and infinite systems

Lucia Reining[1], Silvana Botti[1], A.G. Marinopoulos[1], Valerio Olevano[1],
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Many problems of broad interest (e.g. the understanding of electronic spectra, or the description of certain chemical reactions) involve, or are even based on, electronic excitations. However, today the range of systems for which electronic excitations can be calculated *ab initio*, and the precision that can be reached in these calculations, are much more limited than what they are in the case of ground state calculations. This situation is, at least in part, due to the presence of long-range interactions in the excited state: in a photoemission experiment, for example, an electron is removed and the 1/r potential of the hole has to be dealt with. In an absorption experiment dipoles are created, and besides their interaction also the electron-hole screened interaction has to be treated properly. It is therefore crucial to understand the role of these interactions and find ways to treat them efficiently.

In this talk we will concentrate on absorption and electron-energy loss spectra of both finite and infinite systems. Today, the two main developments for their *ab initio* calculation are, on one side, the solution of the Bethe-Salpeter equation (BSE) [1,2], and, on the other hand, Time-Dependent Density Functional Theory (TDDFT) [3]. Both approaches are promising, but suffer from different shortcomings: the solution of the Bethe-Salpeter equation is numerically very demanding, whereas TDDFT has the problem that a generally valid and tractable approximation to the so-called exchange-correlation kernel f_{xc} has not yet been found.

We will present a general description which puts both the TDDFT and the BSE approaches, and both absorption and loss spectroscopies, on the same footing and facilitates their comparison. This will then allow us to

- discuss why loss spectra in the solid are often well described by TDDFT, whereas absorption spectra are not
- discuss why, on the other hand, TDDFT often succeeds to describe absorption spectra of finite systems
- clarify the role of the crystal local field effects in various circumstances
- finally, derive a new approximation for the TDDFT f_{xc} from the Bethe-Salpeter equation. We show that its long-range behaviour is crucial for a good description of absorption spectra in solids, and, in the case of continuum excitons, even sufficient for reproducing the excitonic effects and yielding excellent agreement between the calculated and the experimental absorption spectra [4].

In order to illustrate these discussions, several systems will be used as examples: atoms, bulk semiconductors, TiO_2 [5] and graphite.

[1] G. Onida, L. Reining, R.W. Godby, R. Del Sole and W. Andreoni, Phys. Rev. Lett. **75**, 818 (1995); S. Albrecht, L. Reining, R. Del Sole, and G. Onida, Phys. Rev. Lett. **80**, 4510 (1998); V. Olevano and L. Reining, Phys. Rev. Lett. **86**, 5962 (2001).

[2] L.X. Benedict, E. L. Shirley, and R. B. Bohn, Phys. Rev. Lett. **80**, 4514 (1998); Phys. Rev. B **57**, R9385 (1998); W.A. Caliebe, J.A. Soininen, E.L. Shirley, C.-C. Kao and K. Hämäläinen,

Phys. Rev. Lett. **84**, 3907 (2000); M. Rohlfing and S. G. Louie, Phys. Rev. Lett. **80**, 3320 (1998); Phys. Rev. Lett. **81**, 2312 (1998).

[3] E. Runge and E. K. U. Gross, Phys. Rev. Lett. **52**, 997 (1984); E.K.U. Gross and W. Kohn, Phys. Rev. Lett. **55**, 2850 (1985); Phys. Rev. Lett. **57**, 923 (E) (1986).

[4] L. Reining, V. Olevano, A. Rubio and G. Onida, cond-mat/0109434.

[5] N. Vast, L. Reining, V. Olevano, P. Schattschneider, and B. Jouffrey, Phys. Rev. Lett. (2002).

The Dynamical Mean Field Theory of Correlated Systems and its implementation in Electronic Structure Calculations

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The Dynamical Mean Field Theory (DMFT) has been developed over the past few years for the quantitative study of strongly correlated electron systems. This approach involves a mapping onto a self-consistent quantum impurity problem. Incoherent and quasi-particle processes are treated on equal footing within DMFT. I will review this approach, as well as its early success in providing a detailed theory of the Mott metal-insulator transition. I will also describe the recent applications of this method in the context of electronic structure calculations of correlated materials (LDA+DMFT), particularly transition metal oxides and f-electron systems.

Nanocrystals under pressure

Carla Molteni

Cavendish Laboratory TCM, University of Cambridge, Great Britain

The study of semiconductor nanocrystals under pressure is uncovering novel mechanisms of phase transformations that shed light on important issues like crystal structure transformations, nucleation phenomena and size dependence. These processes can now be elucidated at the atomistic level by performing simulations with a recently developed constant-pressure molecular dynamics method for non-periodic systems, which combine a classical description of the pressure transmitting medium with a quantum mechanical description of the system of interest [1].

Results will be presented for silicon and CdS nanocrystals, treated within either density functional theory or tight-binding techniques. Pressure-induced structural transformations in silicon nanocrystals of various sizes show common characteristics, with a tendency towards a metallic behavior at high pressure and hysteresis when the pressure is released [2].

[1] R. Martoňák, C. Molteni and M. Parrinello, Phys. Rev. Lett. **84**, 682 (2000).

[2] C. Molteni, R. Martoňák and M. Parrinello, J. Chem. Phys. **114**, 5358 (2001)

Towards Large-Scale Electronic Structure Calculations with Parallel SIESTA

Julian D. Gale,[1] Emilio Artacho,[2] Alberto García,[3] Javier Junquera,[4] Pablo Ordejón,[5] Daniel Sánchez-Portal[6] and José M Soler[7]

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The SIESTA (Spanish Initiaave for the Electronic Structure of Thousands of Atoms) method [1,2] has already been demonstrated to make it feasible to study in excess of a thousand atoms on a single node workstation, and has been used successfully in many applications. Here the parallelisation of the algorithms involved will be presented and discussed in terms of their efficiency, both working within the frameworks of diagonalisation and linear scaling methods for achieving self-consistency. lt will be demonstrated that it is feasible to perform calculations on the order of 105 atoms with present day computers using the SIESTA approach.

[1] D. Sánchez-Portal, P. Ordejón, E. Artacho and J.M. Soler, int. J. Quant Chem., 65, 453 (1997).

[2] E. Artacho, D. Sánchez-Portal, P. Ordejón. A. Garcia, and J.M. Soler, Phys. Stat Solidi (b) 215, 809 (1999).

The physics of the superconducting Fullerenes

Erik Koch and Ole Gunnarsson

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With the recent discovery of superconductivity at 117 K in hole doped C60-2CHBr3, the Fullerenes have started to rival the cuprates for the title “high temperature superconductor”. We give an overview of the rich physics of this class of materials. In particular, we address questions arising from the strong correlation of the electrons: Why they are not Mott insulators and the unusual role that efficient screening plays for the superconductivity in these molecular crystals. In order to handle the strong correlation effects in the Fullerenes we use quantum Monte Carlo methods for generalized Hubbard-Hamiltonians, which we be briefly introduce.

Finally we discuss very recent results concerning the physics of the new C60-based field-effect devices

All-electron magnetic response with pseudopotentials-. EPR g-tensor of defects in solids and NMR chemical shifts.

Francesco Mauri

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Chris J. Pickard

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The orbital magnetic response is at the origin of important physical properties that are exploited to determine the microscopic structure of materials using the electron paramagnetic resonance (EPR) or the nuclear magnetic resonance (NMR). Indeed, the knowledge of the orbital currents linearly-induced by an uniform external magnetic field, allows us to compute two important quantities measured in magnetic resonance spectroscopies: the EPR g-tensor of defects in solids and the NMR chemical shifts. I will present a formalism for the ab initio calculation of all-electron magnetic response in molecules and solids with pseudepotentials, based an density functional theory [1]. So far, derivations of pseudopotential Hamiltonians have not dealt with magnetic fields. To correctly describe the interaction between orbital degrees of freedom and magnetic fields within a pseudopotential approach, we introduce an extension of Blochl's Projector Augmented-Wave (PAW) method, that we call the Gauge Including Projector Augmented-Wave (GIPAW) approach. The knowledge of the induced all-electron current allow us to compute the EPR g-tensor [2] and the induced magnetic field at the nuclear positions, which defines the NMR chemical shift [1]. We successfully validate our theory by comparison with all-electron results. Moreover, we perform the first prediction of EPR g-tensors in the solid state and find the results to be in excellent agreement with experiment for the E't defect center ind the substitutional phosphorus defect centers of quartz [2]. Combined with the calculation of hyperfine parameters we expect that our GIPAW based first principles approach to the prediction of EPR g-tensors will be of great use in the assessment of models proposed for less well characterized paramagnetic defects.

[1] C. J. Pickard, F. Mauri, Phys. Rev. B 63, 245101 (2001).

[2] C. J. Pickard, F. Mauri preprint cond-mat/0110092 (2001)

Study of molecule chemisorption on noble metal surfaces

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Recent experiments with the scanning tunneling microscope (STM) have permitted to measure properies of a single molecule chemisorbed on different nobel metal substrates [1,2]. In particular, the vibrational excitation of certain molecular modes has enabled chemical analysis with the STM, and the tunneling current has also been used to induced localized and controlled reactions. Some theoretical progress has been accomplished on these effects [3]. It has been shown that density functional theory (DFT) as implemented in plane waves pseudopotential codes, is a good starting point to model inelastic effects on chemisorbed systems. In order to achieve a good understanding of the experimental data, an accurate theoretical description of chemisorption is crucial.

The aim of this contribution is to assess the capacity of actual implementations of DFT (the simulation package DACAPO by CAMP, Technical University of Denmark) by studying the chemisorption of different molecular systems and by comparing with the experimental data in the very low coverage limit.

The first system to study is C2H2 on Cu(100), where subsequent stages of dehydrogenation have been accomplished with the STM, hereby furnishing us with a series of reaction fragments with their own STM images, and vibration frequencies. The theory allows us to understand the different fragment chemisorption in terms of the orbitals of each free molecular species, and to evaluate the measured quantities. In this case, the agreement is certainly good and we have a powerful theoretical tool to study these systems.

Another case of interest is the STM-induced dehydrogenation of C6H6 on Cu(100) [2]. Experimentally, the final fragment is supposed to be C6H4. Our preliminary data seem to suggest that C6H5 can also be a final fragment.

Unsaturated hydrocarbon chemisorption seems to be a good system for this kind of DFT studies. The last part of the talk will be devoted to the case of CO/Cu(111), NO/Cu(111), and O2/Ag(110). Despite an overall good agreement with chemisorption energies and electronic properties, a closer look into these systems shows important divergences with experimental data. In particular, the known chemisorption site for CO on noble metal surfaces is not correctly reproduced, the local magnetic moment on NO does not agree with measurements and the vibrational excitation of O2/Ag(110) shows the need for a more accurate electronic structure calculation.

[1] B.C. Stipe, M. A. Rezaei, and W. Ho, Science 280 (1998) 1732.

[2] L. Lauhon and W. Ho, J. Phys. Chem. A. 104, 2463 (2000).

[31 N. Lorente and M. Persson, Phys. Rey. Letters 85 (2000) 2997; N. Lorente, M. Persson, L. Lauhon, and W. Ho, Phys. Rev. Letters 86 (2001) 2593.

Structural relaxations in electronically excited poly(para-phenylene)

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The difference in energy between the absorption and luminescence energies (the Stokes shift) is a manifestation of the structural relaxations which occur in the excited state. We use a combination of GW-BSE, LDA-DFT and tight-binding calculations to investigate these relaxations in poly(p-phenylene) (PPP). The electron-hole interaction mixes in the quasiparticle states at different wave vectors and bands. In this case the mixing of the quasiparticle states is essentially independent of the relaxations. This leads to the conclusión that the relaxations can be accurately modelled without explicitly including the electron-hole interaction. We find that excitons in PPP are self-localized by a local reduction in the angle between monomers. The electron-hole correlation length is about 4-5 monomers, while the structural relaxation takes place over 40-50 monomers.

Exchange-Correlation Energy as a Function of the Orbital Ocupancies: Implementation on First-Principles Local Orbital Methods.

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We introduce a Local Density (LD) formalism where the total energy of the system is obtained as a function of the orbital occupancies, $\{n_{i\sigma}\}$. The exchange energy, $E_x[\{n_{i\sigma}\}]$, is written in terms of the electrostatic interaction between a charge, $n_{i\sigma}$, and its hole, $(1 - n_{i\sigma})$, while the correlation energy is analyzed by means of a generalized Hubbard hamiltonian, using a dynamical mean field approximation. This approximation allows us to calculate the correlation energy, $E_c[\{n_{i\sigma}\}]$, and the corresponding correlation potential, $V_{c,i\sigma} = \partial E_c[\{n_{i\sigma}\}]/\partial n_{i\sigma}$.Once E_c,$V_{c,i\sigma}$,E_x and the exchange potential $V_{x,i\sigma} = \partial E_x[\{n_{i\sigma}\}]/\partial n_{i\sigma}$, are obtained as explicit functions of the orbital occupancies, $\{n_{i\sigma}\}$, our local orbital LD method is completely defined [1]. These ideas can also be applied in a many-body formalism, substitutíng the correlation potential - for a selfenergy, $\Sigma_{c,i\sigma}(\omega)$, calculated within the dynamical mean field approximation.

This LD-approach is applied to several crystals (Si, C, GaN) and molecules (benzene, anthracene, PTCDA), the results showing good agreement with other first-principles methtods. In particular, the Ga 3d-bands in GAN are lower than the N 2s-states, a behaviour that is only reproduced in LDA or GGA calculations when self-interaction corrections are included. Finally, we will also discuss bulk Fe, in order to analyze its magnetic properties. In this case, we have obtained both the LD and the many-body solutions. Our results show that, for Fe, the correlation potential is strong enough to cancel out any magnetic effect associated with the intra-atomic Hubbard interaction, U. We conclude that ferromagnetism in Fe is mainly due to the intra-atomic exchange energy, contributing to the first Hund's rule.

[1] P. Pou et al., Phys. Rev. B **62**, 4309 (2000).

Ab initio calculation of the static dielectric tensor of GaAs/AlAs superlattices

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The size reduction achieved in one, two or three dimensions in heterostructures at the nanoscale level leads to electronic ground and excited states widely different from those of the bulk crystals, and has opened the way to a new generation of optoelectronic and photonic devices. (GaAs)p/(AlAs)p (001) superlattices (SL's) are extensively studied examples. The band-offsets at the interfaces act as effective potential barriers which confine the carriers in one dimension; moreover, the artificially superimposed potential induces a coupling between previously independent bulk states. While the GaAs and AlAs bulk semiconductors present an isotropic optical response, in the GaAs/AlAs SL the lowering in the crystal symmetry gives rise to an optical anisotropy in the real part of the dielectric constant (birefringence) and in the imaginary part (absorption anisotropy or dichroism).

Here, we will present a study of the static dielectric tensr of these system . We have performed ab initio calculations for ultrathin SL's [1] and semi-empirical calculations for larger ones [2]. The ab initio calculations are based on the Time-Dependent Density Functional Theory (TDDFT). We have both included the exchange-correlation kernel in the adiabatic local density approximation (TDLDA.) and neglected it (RPA).

The simple picture of the macroscopic dielectric function being a sum of independent transitions between one-electron states ignores contributions which may be especially important when the scale of the system is reduced and the inhomogeneity of the medium more pronounced. In particular, the crystal local field effects are expected to be relevant, since they reflect the charge inhomogeneity of the responding material. This point turns in fact to be crucial for the explanation of the SL birefringence, as we will illustrate by discussing the following results:

Calculations neglecting local field effects account neither for the experimentally observed value of the static birefringence [4], nor for its decrease with decreasing SL period p, even qualitatively.

The behavior of the dielectric tensor is determined by the equilibrium between quantum confinement and the local fields effects. The use of the effective medium approach [3] is shown to be justified in the growth direction even for small periods, whereas quantum confinement effects are found to be large in the in-plane direction.

The static birefringence is drastically enhanced (up to a factor 7 even for periods as small as p = 8) by the anisotropy of the local fields. Including the latter, the experiment [4] can be reproduced without considering further many body effects.

[1] S. Botti, N. Vast, L. Reining, V. Olevano, L.C. Andreani, to be submitted.

[2] S. Botti and L.C. Andreani, Phys. Rev. B 63, 235313 (2001).

[3] D. Bergman, Physics Report 43, p. 291 (1978); M.G. Cottam and D.R. Tilley, in 'Introduction to surface and superlattice excitations', (Cambridge University Press, Cambridge, 1989), p. 267;

E. Jahne, Phys. Stat. Sol. (b) 194, 279 (1996).

[4] A.A. Sirenko, P. Etchegoin, A. Fainstein, K. Eberl, and M. Cardona, Phys. Rev. B 60, 8253 (1999).

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Hessian model for accelerating ab initio geometry optimizations

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We present two methods to accelerate first-principles structuctural relaxations. In such calculations, the cost of evaluating classical model forces is neglegible compared to that of calculating the true quantum mechanical forces. Thus we use a simple model hessian, obtained from universal first-neighbor harmonic interactions, with fixed stretching and bending constants. Despite its simplicíty, the normal modes of this model hessian represent excellent internal coordinates in molecules and solids, reproducing the long-range acoustic modes. In the first method, the model hessian is used to precondition a conjugate gradients minimization, reducing drastically the effective spectral width and improving greatly the convergence. The same hessian is used in the second method as a starting point in a quasi-Newton algorithm, the modified-Broyden method of Vanderbilt and Louie, in which it accelerates considerable the convergence to the exact hessian. Results of both methods will be presented for geometry optimizations of clusters, slabs and biomolecules.

Two interacting electrons confined in a sphere: some exact and DFT results.

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The problem of two interacting electrons via a Coulomb force and confined in a sphere is exactly solved. Due to the scaling of the matrix elements of the hamiltonian, the interaction between the electrons is more importance the bigger the radius of the sphere is. So, different correlation regimes can be studied by changing the radius R of the well; for small values of R we get the high density limit, where the particles can be considered as nearly independent, whereas larger values of R yield the low density limit, where we have strong correlation between the electrons, being the position of one of the particles strongly determined by the position of the second one.

We have used the Configuration Interaction method, which diagonalizes the hamiltonian matrix of the system in a basis of general linear combinations of Slater orbitals. This method gives a very accurate solution when a sufficiently large configuration basis is employed. Due to the scaling of the matrix elements, the electronic interaction is more importance the bigger the radius of the sphere is.

We have also solved this problem within the DFT, using some of the more usual approximations for the exchange and correlation. The exact treatment of the exchange energy (equivalent to the Hartree-Fock approximation) is also evaluated. We present the energies, probability distributions, densities as well as the DFT potentials: the total effective potential and the contributions of the exchange and the correlation. All these magnitudes clearly show the highly nonlocal properties of the system.

Multilayer nanocrystals in a magnetic field

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The influence of a magnetic field on the electron energy spectra of both uniform and multilayer semiconductor nanocrystals is investigated. The calculations are performed within the kp method and envelope function approximation.

Our calculations reveal that the magnetic field dependence of the energy spectrum varies strongly with the size and compositions of the nanocrystals.

Several interesting phenomena, like spatial polar separation of one-electron charge density and the change of the ground state symmetry with the increase of the magnetic field in quantum dot quantum well structures or rearrangement of some energy levels at B=0 with the increasing thickness of the external shell and crossover from confinement in external shell to internal core under the influence of a magnetic field in quantum dot quantum barrier systems are reported.

Structural properties of glassy and liquid sodium tetrasilicate: comparison between *ab initio* and classical molecular dynamics simulations

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The structural properties of $Na_2Si_4O_9$ in the liquid and in the glassy state are studied by Car-Parrinello molecular dynamics simulations. The results are compared to the structural characteristics obtained by classical molecular dynamics simulations using the Kramer, van Beest and van Santen potential (BKS).

In the $Na_2Si_4O_9$ liquid, the *ab initio* description presents a higher number of defects than the classical description. In particular, comparison between the coordinations, the pair correlation functions and the angle distributions given by the two descriptions will be presented.

In the $Na_2Si_4O_9$ glass, the details of the local structure are found to be different in the ab initio and in the classical descriptions. We will show that these differences are related to the modifications of the atomic charges due to the introduction of Na atoms, which are not taken into account in the classical simulations.

First principles molecular dynamics study of the stretching frequencies of hydrogen molecules in carbon nanotubes.

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We present a study of the vibrational frequencies of hydrogen molecules adsorbed in bundles of single wall carbon nanotubes. The frequencies are extracted from the analysis of first principles molecular dynamics trajectories. We study the case of molecules inside the nanotubes (endohedral), and in the interstitial pores between the nanotubes (exohedral). We find that, in both configurations, the stretching frequencies are red-shifted with respect to the free H_2 molecule. However, whereas all the exohedral molecules exhibit a redshift of around 45 cm^{-1}, the endohedral molecules show two frequencies, one close to that of the exohedral molecules and the other similar to that of free H_2.

The lifetimes of quasi-particle excitations in para- and ferromagnetic transition metals: LMTO GW approach and scattering theory model calculations

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We report theoretical studies of the electron excitation lifetimes in paramagnetic Rh, Pd, Ag and ferromagnetic Fe, Co, Ni by means of the ab initio many-body LMTO GW approach. We show that the spin-averaged ab initio LMTO GW lifetimes in Fe, Co, Ni are in agreement with the available experimental results while the calculated spin-dependent lifetimes deviate from the spin-resolved experimental data. We propose a two-paramete density-of-state convolution model of the scattering theory (STA-DOS) that provides for the momentum- and spin-averaged lifetimes in Rh, Pd, Ag, Co, Ni and Fe a good agreement with the corresponding ab initio results. For the spin-dependent lifetimes in Co, Ni this model leads to much better agreement with experimental results due to taking into account the scattering by the Stoner excitations. For Fe the discrepancy between the theoretical and experimental data is, however, essential, which we refer to the contribution of the spin-wave generation into the damping of excited electrons.

The pressure effect on electronic properties of III-V compounds by semi-empirical tight-binding method

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A semi-empirical tight-binding sp^3s^* method for tetrahedrally co-ordinated cubic materials is used and applied to GaAs, GaSb and GaP to present the electronic band structures. The binary compounds are found to be indirect-gap semiconductor under pressure effect. The ionicity factor under effect of pressure is presented by means of our recent model. The structural phase transition can be seen from the behaviour of the bonding character. The results are compared with the theoretical and experimental data are in reasonable agreement.

Interaction of Light with Clusters within a Real-Space, Real-Time, TDDFT framework

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Time-dependent density functional theory is used, in combination with real space techniques, to calculate various optical properties of a variety of clusters. Simulated processes range from linear optical response, to the non-linear reaction to intense femtosecond laser pulses. In addition, we present an assessment of the quality of several approaches to the exchange and correlation functional which has to be used for this kind of calculations.

Structural and electronic properties of nanosized ferroelectric hybrid structures.

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Hybrid structures including a ferroelectric oxide film surrounded by insulator or metal electrodes [1] are important systems for different technological applications. The miniaturization of the electronic devices encourages the study of the evolution of the ferroelectric properties with thickness as well as mechanical and electrical boundary conditions. Using Density-Functional based methods [2] we have monitored the structural and electronic properties of $BaO/BaTiO_3$, $SrRuO_3/BaTiO_3$, and $Pt/BaTiO_3$ heterostructures, therefore explicitly including the effects of the different chemical environments in the simulations. The atomic relaxation patterns are presented and compared with those obtained for the free-standing $BaTiO_3$ slabs. The band offset for the insulator/ferroelectric interface, as well as the Schottky barriers for the metal/ferroelectric heterojunctions are reported. Finally, the influence of the interface on the dynamical charges of the atoms is discussed, together with the application of the sum rule of Ruini *et al.* [3].

[1] R. A. McKee, F. J. Walker, and M. F. Chisholm, Science **293**, 468 (2001); Th. Tybell, C. Ahn, J. Triscone, Appl. Phys. Lett. **75**, 856 (1999)

[2] We have used the Pseudopotential Plane-wave methodology of the ABINIT package, (http://www.mapr.ucl.ac. and the Numerical Atomic Orbital method, as is implemented in the SIESTA code (J. Soler, E. Artacho, J. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal, submitted to J. Phys. Cond. Matt.; http://www.uam.es/siesta).

[3] A. Ruini, R. Resta, and S. Baroni, Phys. Rev. B, **57**, 5742 (1998)

Theoretical phonon studies of semiconductor structures

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The main goal of the work that we present here is to study the phonon dispersion diagram of several semiconductors, specially of the type III-V (GaAs,GaP, ...) and its alloys MGAX where X=As or P and M are transition metal atoms (Ti,Se, ...) in different proportions.

In a prevíous work [1] our group has demonstrated that this kind of alloys presents an isolated half filled intermediate band. Our final purpose of this work is the calculation of absorptions coefficients for this kind of systems.

In this work we perform accurate calculations of phonon dispersion using the first principles computer code SIESTA [2], within DFT [3, 4] approximation and with LCAO basis set. We use the local density (LDA) and generalized gradient (GGA) approximation for the exchange-correlation potential and norm conserving pseudopotentials for core electrons of all the atoms. SIESTA program builds up the matrix of force constants by calculating forces acting due to small displacements of the atoms.

We use different basis sets to study its effects and comparing them with the experimental results.

References

[1] P. Wahnón and C. Tablero, Phys. Rev. B, submitted

[2] P. Ordejón, E. Artacho and J.M. Soler, Phys. Rev. B 53 (1996) 10441; D. Sanchez Portal, P. Ordejón, E. Artacho and J.M. Soler, Int. J. of Quant. Chem. 65 (1997) 453.

[3] R. G. Parr and W. Yang, Density Functional Theory of Atoms and Molecules, Oxford University Press, Oxford, 1993 .

[4] Electronic Density Functional Theory. Recent Progress and New Directions, Plenum Press, 1998

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Theory of resonant Raman scattering of tetrahedral amorphous carbon

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We present a practical method to compute the vibrational resonant Raman spectra in solids with delocalized excitations. This method tries to go beyond the Placzek approximation aud is valid in the resonant case in solids where excitations are delocalized. This approach is applied to study tetrahedrous amorphous carbon. The vibrational eigenmodes and eigenvalues are determined using density functional theory in the local density approximation and the Raman intensities using a tight binding approximation. The computed spectra are in good agreement with the experimental ones measured with visible and UV lasers.

Ab-initio calculation of ^{17}O NMR spectra in oxides.

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^{17}O NMR spectroscopy is a promising tool for the study of the microscopic structure of oxides. ^{17}O is a quadrupolar nucleus and thus both chemical shift and electric field gradient tensors can be exploited. Due to the oxygen lone pair, the ^{17}O chemical shifts cover a very broad range of 800 ppm. However, the correlations between local structures and NMR parameters are still unknown. Empirical rules are commonly used to extract informations from the raw experimental data. However this approach cannot be applied in the solid state, as the atomic configurations often cannot be modeled by chemical analogues. Ab-initio calculation is the only way to obtain an unambiguous determination of the microspcopic structure. Until recently, the conventional approach to the theoretical interpretation of solid state NMR spectra was to approximate the infinite solid by a cluster [1] but the comparison with experiments is poor. Here we will present results obtained with a new method to simulate periodic solids without the cluster approximation. We apply this recently developed approach for the first principles calculation of NMR chemical shifts [2,3] and electric field gradients, to SiO_2 polymorphs and two zeolites (Faujasite and Ferrierite). The computed NMR parameters are in excellent agreement with the experimental data.

[1] X. Xue and M. Kanzaki, Sol. St. Nucl. Magn. Res. 16, 245 (2000)

[2] F. Mauri, B.G. Pfrommer, and S.G. Louie, Phys. Rev. Lett. 77, 5300 (1996)

[3] C.J. Pickard and F. Mauri, Phys. Rev. B to be published, cond-mat/0101257

A k-space approach to finite electric fields in insulators

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Building upon ideas in a recent paper by Nunes and Gonze,[1] we propose a first-principles approach to study insulators in a finite macroscopic electric field ϵ based on a k-space representation in terms of polarized Bloch-like functions $\mathrm{u}^{\epsilon}_{nk}$. The electric enthalpy functional is written

$$\mathrm{F}[\mathrm{u}^{\epsilon}_{nk}\ ,\epsilon] = \mathrm{E}_0[\mathrm{u}^{\epsilon}_{nk}] - \epsilon.\mathrm{P}_{mac}[\mathrm{u}^{\epsilon}_{nk}]$$

where E_0 is the usual zero-field functional and P_{mac} is the discretized Berry-phase polarization formula for a regular mesh of k points. The functional F has a metastable minimum below a critical field ϵ_c, which depends inversely upon the k-point mesh spacing; the disappearence of the minimum above ϵ_c corresponds to a kind of intrinsic dielectric breakdown. In order to cope with the Berry-phase term in F, which involves couplings between nearby k-points, modifications to the usual iterative minimization procedure are needed. We first apply the method to a one-dimensional tight-binding model, and compare the results with those obtained for the same model using a real-space (Wannier-function) approach.[2] We then discuss the implementation of the method in a standard density-functional electronic-structure code (specifically, ABINIT), and the use of this approach for the computation of dielectric constants and effective charges in tetrahedral semiconductors.

[1] R.W. Nunes and Xavier Gonze, Phys. Rey. B 63, 155107-1 (2001).

[2] R.W. Nunes and David Vanderbilt, Phys. Rey. Lett. 73, 712 (1994)

Silver atoms embedded in ionic lattices

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The presence of neutral silver atoms trapped at cationic sites in LiCl, NaCl and KCl have been proved through Electronic Paramagnetic Resonance. Moreover, an anionic silver center has been detected in KCl. The low concentration of silver impurities does not allow determining experimentally the local geometry relaxation. This relaxation is expected to be large because of the larger size of the Ag0 atom respect to the lattice ions and the lack of electrostatic interaction of Ag0 with the nearest ions. The equilibrium distances of the ground state and the excitation energies of the lowest excited states have been computed using DFT calculations by means of the ADF code. Different cluster models of increasing size (from 7 up to 123 atoms) have been studied to analyze the character of the ground and excited states. Results show that: 1) The large outwards relaxation of ~15-25% around the Ag0 impurity plays an important role to understand the stability of the cationic centers. 2) In KCl, the anionic center is much more stable that the cationic one. Moreover, in the cationic center, the charge of the unpaired electron is more concentrated around the silver atom, in good agreement with experimental results. 4) Large clusters are needed to account for the delocalized character of some excited states. 5) Applied hydrostatic pressures can transform the cationic and anionic Ag0 centers in Ag+ ones, but the mechanism is different in every case.

5.5.2 Report on Workshop “Hands-on-FPLO”

March 3 to 7, 2002, IFW Dresden

Supported by ESF, STRUC-ψ_k Programme

1. Scientific content of the event

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

This package is a Full-Potential Local-Orbital minimum-basis code [1] to solve the Kohn-Sham equations in a regular lattice by using the local density approximation. The situation of a chemically disordered structure is covered by an implemented CPA (coherent potential approximation) solver [2]. Relativistic effects can be treated in a related 4-component code that solves the Kohn-Sham-Dirac equations (RFPLO) [3], and the LSDA+U formalism is currently being implemented. Much effort has been spent in the mentioned methods to achieve a level of numerical accuracy which is comparabel to advanced full-potential LAPW implementations, though the basis set is almost one order of magnitude smaller. In particular, the absolute values of the total energy were found to agree with the results of the FLAPW package WIEN-97 within about 1 mHartree per atom for non-relativistic calculations [1]. The agreement with respect to lattice parameters and bulk moduli is better than within 0.5 and 10 complementary. While WIENxx in most cases still sets the accuracy standard, a major advantage of the FPLO package is its minimum basis concept. It makes highly accurate full-potential calculations for elementary cells of up to 100 transition metal atoms feasible and is a good starting point for approaches beyond the local density approximation.

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

References:

[1] K. Koepernik and H. Eschrig, Full-potential nonorthogonal local-orbital minimum-basis band-structure scheme, Phys. Rev. B **59**, 1743 (1999); I. Opahle, K. Koepernik, and H. Eschrig, Full-potential band-structure calculation of iron pyrite, Phys. Rev. B **60**, 14035 (1999).

[2] K. Koepernik, B. Velicky, R. Hayn, and H. Eschrig, Self-consistent LCAO-CPA method for disordered alloys, Phys. Rev. B **55**, 5717 (1997).

[3] I. Opahle, PhD thesis, TU Dresden 2001 (publication in preparation).

2. Lectures held

... can be found at **http://www/ifw-dresden.de/FPLO/lectures.htm**.

Local lecturers (IFW Dresden)

Prof. Dr. Helmut Eschrig
Dr. Klaus Koepernik
Ulrike Nitzsche
Dr. Manuel Richter
Dr. Ingo Opahle
Igor Chaplygin

Invited lecturers

Dr. M. Kuzmin (Zaragoza, Spain)
Dr. H. Rosner (Davis, USA)
Dr. Martin Divis (Prague, Czech Republic)
Dr. Pavel Novak (Prague, Czech Republic)
Jan Kunes (Prague, Czech Republic)

3. Assessment of the results, contributions to the future direction of the field

As the main result of the workshop, all participants are able to handle the code for routine calculations. The participants further started calculations on systems of their choice. In cases were difficulties with the code handling encountered, they could be solved together with the tutors. Licences to use the code for academic purposes were issued to the home departments of all participants (15 in total), and the updated source code (FPLO-2) was released recently. We believe that the distribution of this efficient and numerically accurate code will considerably enhance the role of DFT calculations for the study of complex materials. We further hope that the use of FPLO will steadily grow in near future (**http://www.ifw-dresden.de/FPLO/pub.htm**). The second workshop “Hands-on-FPLO” is scheduled for March, 2003.

4. Statistical information on participants

Academic level: 14 students, 24 PhD, 3 professors
Countries of origin: 28 Germany, 4 Czech Republic, 2 Spain, 2 USA, 1 Belgium, 1 France, 1 Poland, 1 Algeria, 1 Argentina.
Sex: 36 males, 5 females.

Manuel Richter

5.5.3 Report on the Hands-on CASTEP Workshop

The Nuts and Bolts of First-Principles Simulation
Durham University, December 2001

Supported by the ESF through the $\Psi_{\mathbf{k}}$ Network

Philip Lindan[1], Stewart Clark[2] and Walter Temmerman[3]

Background

These days it seems that everyone wants to do first-principles calculations. The methods grew up in condensed-matter physics circles but in the last few years their capabilities have increased so much that many want to get involved, learn the tricks of the trade and harness these capabilities for their research. First-principles calculations are highly prized in every field where fundamental atomistic knowledge is the currency: nowadays this means biochemistry and electronics as much as it does condensed-matter physics. The majority of new users are not experts in condensed matter theory, and many are experimentalists by trade. There is therefore a high demand for training in the basics and in how to get to grips with real calculations. We organised this workshop in response to this need.

Almost three years ago a group of people[4] embarked on a major project to rewrite `CASTEP` from the ground up (or more accurately from the top down). `CASTEP` was already one of the leading "first-principles" codes, a synonym for DFT calculations employing a plane-wave basis and pseudopotentials. The aim in writing a radically-different, all-new modular code was to create the ideal platform for both efficient calculations and new developments. So, while the need for training in first-principles theory and practise has in any case been growing rapidly, the arrival of a new code made the need even more pressing.

As is usual large meetings are some time in the making: we proposed the idea to $\Psi_{\mathbf{k}}$ in October 2000, targeting the end of 2001. We were fortunate to receive funding of £10,000, and it is worth saying that without such backing this project would never have started.

We chose Durham for two reasons. First, the University offered exceptionally competitive rates and this enabled us to provide support for over 50 young researchers out of a total delegation of 90. Second, Stewart Clark agreed to be local organiser, taking upon himself a huge workload that was crucial to our success.

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[1] University of Kent at Canterbury, Kent CT2 7NR, UK

[2] University of Durham, Durham DH1 3LE, UK

[3] Daresbury Laboratory, Warrington WA4 4AD, UK

[4] The Castep Developers Group (CDG): M. D. Segall (Cambridge), P. D. Lindan (Canterbury), M. J. Probert (York), C. J. Pickard (Cambridge), P. J. Hasnip (Cambridge), S. J. Clark (Durham) and M. C. Payne (Cambridge). Also see *J. Phys. Condens. Matter* **14**, 2717 (2002).

Organisation

The workshop was designed for complete beginners, typically those just starting out on a Ph. D. The workshop spanned a week, starting on the evening of the 6th December 2001 and ending at lunchtime on the 13th. We chose to mix lectures and practical sessions in roughly equal measure, This meant on average four one-hour lectures and four hours of practical work per day. In the initial stages the emphasis was on building up basic knowledge, and the later stages saw more practical work and coverage of more advanced topics. To remind us of our scientific goals we also had two lectures in which themed reviews of research areas were given.

Excluding the lecturers there were 90 participants in total. These came from groups in 10 European countries and 5 countries outside Europe, with more than 25 nationalities represented. There were 60 young researchers in attendance. Financial support was given to 54 participants, while 36 delegates paid a small fee to cover costs.

How did it go?

Who better to ask than the participants themselves? We asked for their opinions *via* an anonymous questionnaire distributed on the penultimate day. The most consistent praise came for the excellent contact with the code developers and experts in the application of first-principles calculations. This gave continual opportunity not only to learn the technicalities of the code but also to understand the simulation-specific scientific thinking that drives applications forward. The latter is vital to success but rarely available from the literature. The lecture programme was also highly praised for its breadth and expert content. However, some participants found certain topics very challenging, which may be traced to the wide participation and background knowledge. This followed through to the practical sessions. These were quite deliberately set up in such a way that the onus was with the participant to develop and explore a theme minimally specified. Our idea was to make the exercises more like mini research projects so as to have the flavour of the "live" research environment. For some this worked very well, as they were confident to draw upon the technical and scientific resources offered by the organisers and developers. It is very difficult to cater for every need when the experience and background knowledge is diverse, therefore there were a few who undoubtedly found this daunting, but with the expertise of the authors of `CASTEP` on hand, many conceptual difficulties in running a first-principles code were overcome. This undoubtedly remains a challenge for future workshops.

We were very pleased with how well the new `CASTEP` code performed considering that at the time it was in beta form. It is a testament to the code design that complete newcomers could quickly start to run "proper" calculations owing to the built-in intelligence and simple input. Of course some bugs emerged, but with at least half-a-dozen experts in the room these were rapidly fixed on the spot! We thank the participants for their patience.

Everyone seemed happy with the venue in general, but inevitably there were some minor hiccups (most of which went un-noticed!). We were only able to have a handful of Materials Studio licenses which were always in demand. We also hope that no-one was too cold, remembering that this was the North of England in winter!

We also think the social side of the meeting was rather successful. We can't claim any credit for this, other than through providing a bountiful welcome evening and an all-conquering pool team.

Perhaps the best indicator that allows us to call the workshop a success was the number of times we were asked "can you do it again please, as soon as possible?".

Working with `CASTEP`

A major goal of this meeting was to see `CASTEP` adopted for use by a wider community. To this end the CDG invited ideas for collaborative work that might lead to new developments going into the code. This will ensure a strong development community with a vested interest in the whole project. Many potential collaborations were identified and are being built up right now. Accelrys, the company that markets the commercial version of `CASTEP` , also helped in this respect by offering free licenses for Materials Studio to cover six months. Most important of all, all Ph. D. students who attended the meeting will be enabled to use `CASTEP` for the duration of their studies.

Summary

We think that most people got most of what they needed from this workshop, which is success by any measure. Some of the programme highlights were:

- Very low cost, many supported students
- Extensive access to the authors of the code and applications experts
- Broad programme of lectures
- A realistic "live" scientific experience
- Informal and inclusive atmosphere

Some of the scientific and technical highlights were:

- Enabling 90 people new to first-principles calculations
- The introduction of a new modular first-principles code
- Non-local exchange-correlation functionals
- Linear response NMR, ESR and phonons
- The formation of many collaborative relationships

Thanks

Our thanks go first and foremost to $\Psi_{\mathbf{k}}$ for funding this workshop. We are also deeply indebted to the lecturers who not only prepared and gave excellent talks, but also spent many hours talking to participants and giving freely of their expertise. Many thanks go to all local organisers: Stewart Clark, Sharon Fairless the secretary, and the helpful PhD students (Philip Rushton and Paul Tulip), to Durham University and Grey College, and to the participants for their enthusiastic involvement.

Lecturers

Technical

Stewart Clark, University of Durham
Mike Gillan, University College London
Phil Hasnip, University of Cambridge
Philip Lindan. University of Kent at Canterbury
Mike Payne, University of Cambridge
Chris Pickard, University of Cambridge
Matt Probert, University of York
Keith Refson, CLRC Rutherford Laboratory
Matt Segall, University of Cambridge

Research applications

David Bird, University of Bath
Mike Finnis, Queens University Belfast

Commercial

Xenophon Krokidis, Accelrys
Klaus Stark, Accelrys

Programme

Thursday 6th December

14.00 Registration
19.00 Welcome Reception - Grey College JCR

Friday 7th December
(3 Morning Lectures, 2 Afternoon Lectures and Workshop)

09.00 LECTURE 1 Computational materials science: an overview
Mike Payne, University of Cambridge

10.00 LECTURE 2 The modellers perspective: philosophy and ingredients of atomic-scale modelling

Philip Lindan. University of Kent at Canterbury

11.00 COFFEE

11.30 LECTURE 3 The outline of DFT and the LDA
Mike Gillan, University College London

12.30 LUNCH

14.15 LECTURE 4 Introduction to CASTEP: history, design, features, control
Matt Segall, University of Cambridge

15.15 LECTURE 5 Introduction to the materials studio interface, plus enough to get CASTEP running
Xenophon Krokidis, Accelrys

16.15 COFFEE

16.15 WORKSHOP Introduction to the CASTEP code and interface

18.30 DINNER

Saturday 8th December
(3 Morning Lectures, 2 Afternoon Lectures and Workshop)

09.00 LECTURE 6 Supercells, plane waves, bands, k-points and symmetry
Matt Segall, University of Cambridge

10.00 LECTURE 7 Pseudopotentials I: local and non-local NC, generation and testing
Chris Pickard, University of Cambridge

11.00 COFFEE

11.30 LECTURE 8 Finding the ground state: simple approaches
Phil Hasnip, University of Cambridge

12.30 LUNCH

14.15 LECTURE 9 Is it running properly? What does the output mean?
Philip Lindan, University of Kent at Canterbury

15.15 LECTURE 10 Testing, testing: basic procedure to validate calculations
Keith Refson, CLRC Rutherford Laboratory

16.15 COFFEE

16.15 WORKSHOP More involved setting up, determining cut-offs, evaluating a pseudopotential, simple materials properties

18.30 DINNER

Sunday 9th December
(3 Morning Lectures, 2 Afternoon Lectures and Workshop)

09.00 LECTURE 11 Pseudopotentials II: ultrasoft, PAW, self-consistent
Chris Pickard, University of Cambridge

10.00 LECTURE 12 Band structure calculations
Stewart Clark, University of Durham

11.00 COFFEE

11.30 LECTURE 13 Gradient corrections, other functionals
Stewart Clark, University of Durham

12.30 LUNCH

14.15 LECTURE 14 Forces and stresses
Matt Probert, University of York

15.15 LECTURE 15 Structural calculations and pressure: the total energy approach
Matt Probert, University of York

16.15 COFFEE

16.15 WORKSHOP Structure calculations

18.30 DINNER

Monday 10th December
(3 Morning Lectures and Afternoon Outing)

09.00 LECTURE 16 Metals and EDFT
Phil Hasnip, University of Cambridge

10.00 LECTURE 17 Electronic properties: magnetism and optical properties
Chris Pickard, University of Cambridge

11.00 COFFEE

11.30 LECTURE 18 A first look at MD
Matt Probert, University of York

12.30 LUNCH

FREE AFTERNOON

18.30 DINNER

Tuesday 11th December
(3 Morning Lectures and Afternoon Workshop)

09.00 LECTURE 19 Overview of MD applications
Keith Refson, CLRC Rutherford Laboratory

10.00 LECTURE 20 Catalysis and interfaces
Mike Finnis, Queens University Belfast

11.00 COFFEE

11.30 LECTURE 21 Surfaces and molecules
David Bird, University of Bath

12.30 LUNCH

14.15 WORKSHOP Metals, surfaces and MD

16.00 COFFEE

18.30 DINNER

Wedneday 12th December
(3 Morning Lectures and Afternoon Workshop)

09.00 LECTURE 22 Linear Response: Theory
Philip Lindan, University of Kent at Canterbury

10.00 LECTURE 23 LRT: calculating phonon dispersion relations
Stewart Clark, University of Durham

11.00 COFFEE

11.30 Open Question and Answer Session about running CASTEP
All Lecturers

12.30 LUNCH

14.15 WORKSHOP Parallel sessions for all applications

16.00 COFFEE

19.15 Drinks, Grey College JCR

WORKSHOP DINNER

Thursday 13th December
(3 Morning Lectures and CLOSE)

09.00 LECTURE 24 DFT plane-wave PP versus other approaches
Mike Payne, University of Cambridge

10.00 LECTURE 25 Obtaining the code: playing your part in development
Mike Payne, University of Cambridge

11.00 COFFEE

11.30 LECTURE 26 Upcoming developments and the future for DFT
Mike Payne, University of Cambridge

12.30 LUNCH

14.15 CLOSE OF WORKSHOP

List of participants

Alexander S. Cote	Salford University
Andriy Nevidomskyy	Cavendish Laboratory, University of Cambridge
Brent Walker	University of Cambridge
Bruno Biehler	Bristol
Caroline Jee	Queen Mary, University of London
Charles Bird	University College London
Chi-Cheng Lee	Tamkang University
Chris Cooper	Cardiff University
Christopher Neville-Smith	University of Durham
Clare Clark	University of Cambridge
Daniel Wilson	The Royal Institution of Great Britain
Elizabeth Duplock	University of Kent at Canterbury
Elizabeth Escamilla Roa	CSIC
Hector Mera	University of York
Hong-Liang Shih	Taiwan
Hsin-Yen Chen	Taiwan
Hugh Christopher Greenwell	University of Cambridge
Ian Timothy Cook	AWE
Jonathan Neville	Univ. of Wales
Jonathan Yates	University of Cambridge
Juan Amir	Eindhoven
Kris Delaney	University of York
Lisa Moore	The Queen's University of Belfast
Manisha Mistry	Royal Institution of GB
Matthew Glover	University of York

continued...

Murshed Siddick	University of Edinburgh
Neil Polwart	Heriot Watt University
Paolo Avalle	University of Durham
Paul Peacock	Cambridge University
Pepa Cabrera Sanfelix	Liverpool
Philip S. Smith	University of Durham
Rachel Strong	Cambridge
Riad Shaltaf	Turkey
Sally Birse	University of Cambridge
Sian Joyce	University of Cambridge
Stephen Ball	Liverpool
Tan Feng	Queen Mary, University of London
Tom Archer	University of Cambridge
Yarub Al-Douri	University of Sidi-Bel-Abbes
Zhipan Liu	Queen's University of Belfast
Ahlam Abd El-Monem Ahmed El-Barbary	Sussex University
Alexander Barashev	The University of Liverpool
Alfred Gil Arranz	Facultat de Quimica, Univ. Rovira I Virgili
C. Ignacio Sainz-Diaz	Fac. De Ciencias, CSIC/Universidad de Granada
Carmen Domene	University of Oxford
Christian Huber	Germany
Christian Tuma	Humboldt-Universitaet Berlin
Dominik Legut	Academy of Sciences of the Czech Republic
Giuseppe Pellicane	Universita degli studi di Messina
Hiroshi Yukawa	Nagoya University
Ito Chao	Academia Sinica
Iwona Mroz	University of Wroclaw
Jacqueline Cole	University of Cambridge
Jey-Jau Lee	University of Durham
John Tatini Titantah	University of Antwerpen
Jyh Shing Lin	Tamkang University
Leon Zingales	Univ. Degli Studi di Messina
Marek Hytha	University of Kiel
Maria Ganchenkova	Moscow Eng. Phys. Institute
Mark Calleja	University of Cambridge
Matt Tucker	University of Cambridge
Mattias Forsblom	KTH, SCFAB, Sweden

continued...

Nihed Chaabane	Ecole Polytechnique, France
Peter Bokes	York
Peter Cumpson	National Physical Laboratory
Phuong Yen Ghi	University of Durham
Professor Jiann Lin	NCUE, Taiwan
Professor Lawrence J. Dunne	South Bank University
Professor Ming-Hsien Lee	Tamkang University
Sayede Adlane	Universite d'artois, Faculte Jean Perrin
Sayede Adlane Djamel Eddine	Djilaly Liabes University of Sidi Bel Abbes, Algeria
Shyong Kuan Chen	Taiwan
Stefaan Cottenier	Inst. Voor Kernen Stralingsfysica, Belgium
Tang Li-Chuan	National Chiao-Tung University
Ta-Ya Chu	Academia Sinica
Tina Marie Briere	Tohoku University, Japan
Tomasz Ossowski	Institute of Experimental Physics, Poland
Ute Hantsch	CAU Kiel, Germany
Veronika Brazdova	Humboldt University, Berlin
Vicente Timon Salinero	CSIC, Spain
Yan Song	Queen Mary, University of London
Yi Liu	Graduate School of Engineering, Nagoya University
Yuri Mitrokhin	Udmurt State University, Russia
Yuri Osetsky	The University of Liverpool
Zhang Changjun	University of Kent at Canterbury

5.6 ESF Workshops Announcements

5.6.1 CECAM Psi-k WORKSHOP

Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials

CECAM

Ecole Normale Superieure de Lyon, 46 Allee d'Italie, 69364 Lyon, FRANCE

Monday 23rd September - Wednesday 25th September, 2002

http://www.fisfun.uned.es/ athaesos/

While structural properties of materials are mainly determined by the static electronic ground state, the response to external probes in modern nondestructive spectroscopies must be explained in terms of dynamic excitations. The knowledge of excited states is a fundamental step for the design of materials for technological or medical applications, since it is intimately linked with experimental characterisation. The aim of this workshop is to assess the present status of ab initio approaches for the spectroscopic properties of finite and infinite systems, to establish links between scientists from different communities working on excited states, and to develop and promote new solutions.

Organisers:

Pablo GARCA-GONZLEZ (Universidad Autnoma de Madrid)
Maurizia PALUMMO (Universit di Roma "Tor Vergata")
Olivia PULCI (Universit di Roma "Tor Vergata")
Arno SCHINDLMAYR (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin)
Nathalie VAST (Ecole Polytechnique, Palaiseau)

For further information including details about the registration procedure please visit the workshop homepage

http://www.fisfun.uned.es/ athaesos/.

The deadline for abstract submissions is 21 June 2002.

5.6.2 Workshop on THE DIFFUSION QUANTUM MONTE CARLO METHOD

CECAM, Lyon, France

Thursday 19th to Saturday 21st September 2002

The workshop is jointly funded by CECAM and ESF under its Psi-k program

The list of speakers will include:

S. Fahy
R. Assaraf
L. Mitas
D. Alfe
M. Caffarel
I. Stich
H.-J. Flad
P. Ballone
C. Umrigar
A.J. Williamson
S. Moroni
E. Koch
A. Luchow
S. Baroni
F. Schautz
P. Nightingale
W.M.C. Foulkes

The number of places at this workshop is limited, but those interested in attending should e-mail: qmc-workshop@phy.cam.ac.uk

The webpage for the workshop is:

`http://www.tcm.phy.cam.ac.uk/qmc_workshop/`

and more information will appear there soon.

Organisers:

Richard Needs
Claudia Filippi
Mike Towler

5.6.3 Swedish Summer School on Magnetism

Backagården, Höör, Sweden, 1-5 July, 2002

http://www.backagarden.se

Organizers: Olle Eriksson, Susanne Mirbt and Raquel Lizarraga
Uppsala University, Sweden
Peter Mohn
Technical University of Vienna, Austria

Sponsored by

ESF Psi-k Programme

The programme of the school will cover four topics: thin film magnetism, magnetic semiconductors, magnetic circular xray dichroism (MCXD) and transport properties. Several internationally recognized experts in these fields will be invited to give two hour lectures on experimental and theoretical aspects of the different topics of the conference. The conference will be held in the close vicinity of MAX lab (the conference site is at Backagråen in the Lund area see www.backagarden.se) and is organized by Uppsala University, Lund University and MAX lab. In addition, the school follows directly after the large meeting: nano7/ECOSS21 on June 24-28 in Malmö. Registration via email to Raquel.Lizarraga@fysik.uu.se.

Deadline for registration: June 21, 2002

Programme

Monday, 1 July (Chair: Susanne Mirbt)

09.00-09.15 Olle Eriksson Welcome

09.00-11.00 Hartmut Zabel, Bochum: "Experimental techniques of thin film magnetism"

11.00-13.00 M. Tsoi, Grenoble: "Current induced excitation of spin-waves"

13.00-15.00 Lunch

(Chair: Olle Eriksson)

15.00-17.00 A. Fert, Thales: "Spin-injection: recent experiments"

17.00-19.00 Lars Samuelson, Lund: "Quantum-dot physics, an experimental overview"

19.00 Dinner

Tuesday, 2 July (Chair: Mike Brooks)

09.00-11.00 Jürgen Kirschner, Halle: "Thin film magnetostriction"

11.00-13.00 Stefan Blügel, Jülich: "Theory of thin film magnetism"

13.00-15.00 Lunch

(Chair: Stefan Blügel)

15.00-17.00 N. Garcia, CSIC: "Spin-transport in magnetic nanocontacts"

17.00-19.00 Dimitri Arvanitis, Uppsala: "XMCD and thin film magnetism"

19.00 Dinner

Wednesday, 3 July (Chair: Olle Heinonen)

09.00-11.00 Mike Brooks, Karlsruhe: "Theory of XMCD"

11.00-12.00 Nils Mrtensson, Uppsala: "Strategies and future of magnetism at MAX" lab.

12.00-13.00 Frederic Nguyen-Van Dau, Thales Lab.: "Applications of spin-electronics"

13.00-15.00 Lunch

(Chair: Hartmut Zabel)

15.00-16.00 Susanne Mirbt, Uppsala, Sweden: "Theory of magnetic semiconductors"

16.00-18.00 Panagiotis Poulopoulos, Berlin: "Experimental results of magnetic properties of thin films"

18.00-19.00 Janusz Sadowski, MAX Lab.: "Growth of magnetic semiconducting films"

19.00 Dinner

Thursday, 4 July (Chair: J.Schoenes)

09.00-11.00 Björgvin Hjrvarsson: "Growth and characterization of thin films"

11.00-13.00 Olle Heinonen, Seagate: "Industrial aspects of magnetic semiconductors"

13.00-15.00 Lunch

(Chair: B.Hjrvarsson)

15.00-17.00 N. Papanikolaou, Jülich: "Theory of spin-transport"

17.00-19.00 Joachim Schoenes, Braunschweig: "Magneto-optics"

19.00 Dinner

5.6.4 Sardinia Workshop

The Physics Department, Universitá di Cagliari, and the Cagliari Research Unit of Istituto Nazionale per la Fisica della Materia

organize the

HLCS - EUROCONFERENCE: XII WORKSHOP ON COMPUTATIONAL MATERIALS SCIENCE

23 - 29 September 2002

Sofitel Timi Ama, Villasimius (CA), Sardinia, Italy
web page: http://www.dsf.unica.it/CMS2002

e-mail: workshop@dsf.unica.it
with the sponsorship of

European Commission-Community Research High-Level Scientific Conferences

and

European Science Foundation Programme "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces"

under the patronage of UNESCO

An international workshop on computational techniques and applications to materials science

FORMAT: About 20 invited lectures plus TALK (about 12) and POSTER contributed session.

VENUE: Sofitel Timi Ama at Villasimius (CA), an attractive sea resort on the south-eastern coast of Sardinia, providing comforts and an informal atmosphere.

CONTACT: For scientific and logistic queries: workshop@dsf.unica.it

CONTRIBUTIONS AND PROCEEDINGS: Contributions in poster format are invited. ALL contributions (after refereeing) will be published in a special issue of the journal Computational Materials Science. Deadline for abstract submission: July 31, 2002. Contact V. Fiorentini at +39 070 6754912 or P. Ruggerone at +39 070 6754847 or at workshop@dsf.unica.it for further details. Camera ready manuscripts will be due at the Workshop. LaTeX templates can be downloaded from the workshop homepage: http://www.dsf.unica.it/CMS2002.

INVITED SPEAKERS

P. Carloni (Triest, Italy)
A. Eichler (Wien, Austria)
M. Fanciulli (Agrate, Italy)
V. Fiorentini (Cagliari, Italy)
C. Foerst (Wien, Austria)
E. Gratton (Urbana, USA) (*)
P. Jensen (Lyon, France)

H. Jonsson (Seattle, USA)
G. Lattanzi (Berlin, Germany)
A. Rubio (Valladolid, Spain)
G. Santoro (Triest, Italy)
E. Tadmor (Haifa, Israel) (*)
A. Zunger (Golden, USA) (*)

(*) not yet confirmed

REGISTRATION

The REGISTRATION form can be sent directly from the Workshop homepage

(http://www.dsf.unica.it/CMS2002).

The deadline is June 30, 2002.

The registration should be accompanied by payment receipt of the CONFERENCE FEE (by FAX: ++39-070-510171). The fee includes shuttle services (23/9 Cagliari Airport-Hotel, 29/9 Hotel-Cagliari Airport), half-board lodging at Hotel Sofitel Timi Ama from 23/9 to 29/9, coffee breaks, refreshments, and amounts to

Single room	Euro 960/person
Double room	Euro 700/person
Triple room	Euro 600/person

PAYMENT should be effected by bank money transfer on the bank account # 22698 of Comitato Organizzatore di Attivitá di Fisica Computazionale, at Banco di Sardegna (Swift code: SARDIT3S100), Sede di Cagliari, Codice ABI 1015/7 - CAB 04800.

No fee is requested from the invited speakers.

The Organizing Committee is able to offer support (from 50 % up to 100 % of the conference fees plus travel costs in some cases) to a limited number of young scientists, preferrably PhD students. The deadline for the request of financial support is June 15, 2002. The committee will comunicate its decision on June 25, 2002.

Series Chairman : prof. A. Baldereschi - EPFL Lausanne
Workshop Chairman : prof. F. Meloni - INFM and Universitá di Cagliari
Scientific Secretariat: dr. V. Fiorentini & dr. P. Ruggerone - INFM and Universitá di Cagliari

6 General Workshop/Conference Announcements

Second Announcement and Call for Papers

6.1 ESCM2002: Electronic Structure and Computational Magnetism

http://cmpweb.ameslab.gov/escm2002

15-17 JULY, 2002

Washington, DC

ORGANIZING COMMITTEE:

B.N. Harmon, Ames Laboratory
A.Y. Liu, Georgetown University
D.A. Papaconstantopoulos, Naval Research Laboratory
D.J. Singh, Naval Research Laboratory
G.M. Stocks, Oak Ridge National Laboratory

SCIENTIFIC ADVISORY COMMITTEE:

O.K. Andersen (Germany)
W.H. Butler (U.S.A.)
R.W. Chantrell (U.S.A.)
A.J. Freeman (U.S.A.)
B.L. Gyorffy (U.K.)
M. Jarrell (U.S.A.)
B. Johansson (Sweden)
M.I. Katsnelson (Russia)
B.M. Klein (U.S.A.)
B. Lengsfield (U.S.A.)
A.I. Lichtenstein (Holland)
A.H. MacDonald (U.S.A.)
I.I. Mazin (U.S.A.)
A.J. Millis (U.S.A.)
T. Oguchi (Japan)
G.A. Sawatzky (Canada)
K. Schwarz (Austria)
W.M. Temmerman (U.K.)

We are pleased to announce the conference, "ESCM2002: Electronic Structure and Computational Magnetism", which will be held July 15-17, 2002 on the campus of Georgetown University. This is the second in the ESCM (following ESCM2000, http://cst-www.nrl.navy.mil/escm2000). Details regarding abstract submission and registration are posted on the conference web site (http://cmpweb.ameslab.gov/escm2002). At this time, we invite participants to submit abstracts. In keeping with the tradition of this series a substantial number of additional invited speakers will be selected from the contributed abstracts.

The goal of the conference is to bring together experts and students to discuss the electronic theory of magnetism and magnetic materials as well as couplings from the atomic to the micromagnetic length scale. Some topics of interest are:

- Coupling Length Scales: Atoms to Micromagnetics
- Domain wall structure and interactions

- Non-Collinear Magnetism
- Magnetic anisotropy
- Nano-structured magnets
- Spin Dynamics
- Magnetic Semiconductors
- Rare-Earth and Actinide Magnetism
- Half-Metals
- Molecular Magnets
- Magnetic Excitations
- Spin-Polarized Transport
- Strong Correlations and Magnetism
- Magnetism and Superconductivity

Confirmed speakers so far include:

V.N. Antonov
S. Blugel
G. Brown
W.H. Butler
R.W. Chantrell
R. de Groot
H. Ebert
S. Erwin
H. Eschrig
B. Gyorffy
M.I. Katsnelson
D.I. Khomskii
G. Kotliar
W.R.L. Lambrecht
D.P. Landau
A.I. Lichtenstein
L. Nordstrom
A.P. Mackenzie
M.R. Pederson
L. Sandratskii
T. Schulthess
J.B. Staunton
M. Troyer
J. Mathon
C.J. Lambert
P. Blaha

We hope to have substantial participation by young scientists. To this end the costs for registration and housing will be very moderate, and additionally we expect to subsidize a number of the student and postdoctoral attendees.

We look forward to seeing you in Washington this summer.

6.2 WIEN2002 Workshop

The WIEN2k Development Team and the Materials Simulation Center at Penn State are happy to announce:

WIEN2002: Hands on Workshop on the WIEN2k package
July 22-25, 2002, Penn State University, University Park, PA, USA

The first US workshop on the WIEN code is a hands-on activity dedicated to teach the use of the WIEN2k Density Functional Theory Package. WIEN2k is one of the most popular electronic structure codes used to perform calculations with the Full Potential LAPW method. The workshop is a unique opportunity to learn the use, power and limitations of the package with the tutoring of the authors and developers of the code. The activities will be aimed at graduate students and researchers from industry and academia. The only pre-requisite is to have a basic knowledge of solid state physics, and chemistry. It is planned as a four-day activity with lectures on the scientific aspects of the method, applications, hand-on activities on selected examples, and the opportunity to receive a head start on a personal project.

The invited speakes list includes:

- C. Ambrosch-Draxl
- P. Blaha
- J. Luitz
- G. Madsen
- K. Schwarz
- D. J. Singh

Chair: J. O. Sofo

For more information see http://www.msc.psu.edu.

6.3 IWOSMA2 Workshop

First Announcement

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

October 14-15, 2002, San Srancisco, CA

The second IWOSMA meeting will be held on October 14 and 15, 2002, in the East Bay Area near San Francisco, CA, USA. This continues the series begun in June of 1999 at Daresbury Laboratory, Warrington, UK.
(Please see: `http://srs.dl.ac.uk/msg/MSG_Events_IWOSMA.html`)
The IWOSMA meeting will immediately follow the Users Meetings at the Stanford Synchrotron Radiation Laboratory (SSRL), on October 7-9, and at the Advanced Light Source at Berkeley, on October 10-12. Further information concerning registration, abstract submission, lodging and other specifics will follow in subsequent announcements.

Chair:	J.G. Tobin, LLNL
Co-Chair:	D.K. Shuh, LBNL
Past Chairs:	G. van der Laan and W.M. Temmerman

6.4 Workshop in San Sebastian

”Towards Atomic Scale- and Time-resolution at Interfaces”

1-5 July 2002, San Sebastian

Organizers:

Pedro Miguel Etxenike and Angel Rubio
University of the Basque Country, UPV/EHU, DIPC
http://dipc.ehu.es/arubio/

Aims: The aim of this workshop is to bring together researchers with backgrounds in theory and experiments in order to assess the present state of our understanding of ultrafast phenomena and atomic control at interfaces in condensed matter, surface science, chemistry, and biology. The idea is to contrast both theoretical and experimental studies to gain insight and establish new links and future collaborations. This workshop will be of special interest to researchers conducting theoretical or experimental studies on electron/ion dynamics in

- surfaces - catalysis - molecular electronics - semicondutors - biophysics, etc.

The participation of PhD students and post-docs is strongly encouraged. (The size of the workshop will be around 50 participants).

Preeliminary Programme

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Saturday 29th June
Arrival at San Sebastian/Donostia, Costa Vasca Hotel

Sunday 30th June
Guided Visit of the Guggenhein Musseum

Monday 1st July

08.30-09.30  Registration

09.30-10.00  Opening session: P.M. Echenique

10.00-10.45  "Scanning tunneling microscopy as local probe of electron
              density and dynamics"
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Prof. K. Kern

10.45-11.15 Cofee Break

11.15-12.00 "Probing Electron Dynamics with STM"
Prof. R. Berndt

12.00-12.45 "The scanning tunneling microscope as operative tool:
Physics and chemistry with single atoms and molecules"
Prof. Karl-Heinz Rieder

13.00-16.00 Lunch

16.00-16.45 "Femtosecond Processes in Primary Photosynthesis:
Reactions Optimized for Highest Efficiency"
Prof. W. Zinth

16.45-17.30 "Selective bond breaking in adsorbates by core excitations"
Prof. D. Menzel

17-30-18.00 Cofee Break

18.00-18.45 The core level clock in free molecules and in adsorbates
Dr. Z.W. Gortel

18.45-19.30: "Laser induced charge - transfer processes at adsorbate/
metal interfaces"
Prof. Angel Gonzalez Urena

20.30 Dinner

Tuesday 2nd July

09.30-10.15 "Ultrafast control of bond breaking in photodesorption
from oxide surfaces"
Prof. Hajo Freund

10.15-11.00 "Surface knowledge from ultra-high vacuum to technically-relevant conditions: the example of catalytic CO oxidation"
Dr. Karsten Reuter

11.00-11.30 Cofee Break

11.30-12.15	"Ultrafast charge transfer processes at adsorbates investigated using the core level clock" Prof. Wilfried Wurth
12.15-13.00	"Femtochemistry and ultrafast electron dynamics at adsorbate/ metal interfaces" Prof. Martin Wolf
13.00-16.00	Lunch
16.00-16.45	"Surface dynamics studied with femtosecond vibrational spectroscopy" Dr. Mischa Bonn
16.45-17.30	"Theory of single molecule vibrational spectroscopy and microscopy" Prof. Mats Persson
17.30-18.00	Cofee Break
18.00-19.00	Poster session
20.30	Dinner

Wednesday 3rd July

09.30-10.15	"Atomic-scale control of electronic and dynamical processes on semiconductor and insulator surfaces" Dr. G. Dujardin
10.15-11.00	"Inelastic mean free path for electrons : Ballistic Electron Emission Microscopy" Prof. F. Flores
11.00-11.30	Cofee Break
11.30-12.15	"Scanning tunneling spectroscopy and microscopy of ultrathin dielectric films" Prof. Wolf-Dieter Schneider
12.15-13.00	"Time-resolved photoemission studies of charge-carrier dynamics in the vicinity of the Fermi level"

Dr. Tobias Hertel

13.00-16.00 Lunch

16.00-16.45 "Ultrafast transport phenomena in metal-insulator-metal contacts"
Prof. Walter Pfeiffer

16.45-17.30 "Photoinduced processes at nanoparticulate systems"
Prof. Katharina Al-Shamery

17.30-18.00 Coffe Break

18.00-18.45 "Fs spectroscopy at the planned BESSY SASE FEL"
Prof. Dr. Wolfgang Eberhardt

18.45-19.30 "Combining femtosecond lasers with Scanning Tunneling Microscopy"
Prof. Tony Heinz

19.30 "Roundtable discussion on the new FP6 program of the EC (?)"

21.00 CONFERENCE DINNER

Thursday 4th July

09.30-10.15 "Femtosecond dynamics of electrons at surfaces"
Prof. Thomas Fauster

10.15-11.00 "Effects of adsorbates on image states at metal surfaces"
Prof. J.P. Gauyacq

11.00-11.30 Cofee Break

11.30-12.15 "Probing nanomagnetism on the femtosecond time scale"
Prof. H. A. Durr

12.15-13.00 "Ultrafast relaxation of electrons in metals in space,
time, frequency domains"
Prof. Hrvoje Petek

13.00-16.00 Lunch

16.45-17.15 "Surface state width on noble metal (111) surfaces"

Prof. Stefan Hufner

17.15-18.00 "Momentum Resolved Electron and Phonon Contribution to the Quasiparticle Decay at Metal Surfaces"
Prof. E. Chulkov

18.00-18.30 Cofee Break

18.30-19.15 "Electron phonon contribution to the lifetime of surface states"
Asier Eiguren

19.15-20.00 "Towards theoretical understanding of nanoscale materials functioning and biomolecular processing"
Prof. T. Frauenheim

20.00 Closing remarks

21.00 Dinner

Friday 5th July

Departure

6.5 13th Summer School in Computing Techniques in Physics

"Parallelization of Algorithms in Physics"
Trest, Czech Republic, September 16 - 21 2002

Full details regarding registration, etc are available at:

http://www.fzu.cz/activities/schools/epsschool/

Programme

Jaroslav Nadrchal, *Institute of Physics, Academy of Sciences, Praha, Czech Republic*: "Architectures of Parallel Computers".

Michael Resch, *University of Stuttgart*: "Parallel Programming Models".

Mark Bull, *University of Edinburgh, UK*: "Parallel Programming with Open MP".

Michael Resch, *University of Stuttgart*: "Basics of MPI".

Jrg Hutter, *University of Zurich, Switzerland*: "Car-Parrinello Molecular Dynamics (The CPMD Program Package)".

Thomas Lippert, *University of Wuppertal, Germany*: "Parallelization of the Hybrid Monte Carlo Algorithm for the Study of Sea Quark Physics".

Anthony D. Kennedy, *University of Edinburgh, UK*: "Computational Quantum Field Theory".

Godehard Sutmann, *Research Centre, NIC, Juelich, Germany*: "Large Molecular Dynamics Computer Simulation".

Dieter Kvasnicka, *Technical University Vienna, Austria*: Vienna Program

Rainer Spurzem, *Astronomical Computing Institute, Heidelberg, Germany*: "Computer Simulations in Astrophysics".

The School

The School will be held and all participants will be accommodated in a baroque castle that was recently rebuilt and modernized by the Academy of Sciences of the Czech Republic and offers a very pleasant environment for scientific meetings.

The Location

Trest is a small town (150 km from Prague) in a mild and romantic environment of Bohemian-Moravian Highlands next to the famous splendrous Renaissance town Telc (on the UNESCO list for its uniquely preserved medieval urban architecture).

6.6 Fourth Summer School of the European Mineralogical Union

”Energy Modelling in Minerals”
Budapest, 30 June - 5 July, 2002

We are pleased to announce the Fourth Summer School of the European Mineralogical Union on ”Energy Modelling in Minerals”. The school is being organised by Prof. Carlo Maria Gramaccioli (Milano) and Prof. Tamas Weiszburg (Budapest) and will take place in Budapest between 30 June and 5 July.

The school will concentrate on various techniques for modelling minerals, their properties and structures, as well as some interesting applications of these techniques. A firm link will be established between the theory and experiment (X-ray diffraction, vibrational spectroscopy, neutron scattering, calorimetry). The theoretical methods covered will include quantum-mechanical and semiclassical simulations, lattice dynamics, molecular dynamics, reverse Monte Carlo methods, and Landau theory. The latest applications of these methods to studies of the dynamics of crystal structures, phase transitions, thermodynamics, and geophysics will be presented. The School welcomes equally well participants from the geological, physical, or chemical backgrounds.

The following lectures will be given:

1. J.Ganguly (*University of Arizona, USA*)
   ’Diffusion Processes in Minerals: Fundamental Principles, Experimental Studies and Applications to Natural Processes’
2. A.Navrotsky (*University of California at Davis, USA*)
   ’Thermochemistry, Energetic Modeling, and Systematics’
3. A. Oganov (*University College London, UK*)
   ’Equations of state of solids’
   ’Ab initio theory of phase transitions and thermoelasticity of minerals’
4. S. Ghose (*University of Washington, Seattle, USA*)
   ’Lattice Dynamics, Inelastic Neutron Scattering and Thermodynamic Properties of Minerals’
5. A.Pavese (*Universitá di Milano, Italy*)
   ’Vibrational symmetry and spectroscopy’. (2 lectures)
6. M.Catti (*Universitá di Milano Bicocca, Italy*)
   ’Quantum-mechanical simulations of the high-pressure behaviour of crystals’
7. V.Urusov (*Moscow State University, Russia*)
   ’Atomistic modelling of structure and properties of minerals by minimization of atomization energy’

8. R.Catlow (*The Royal Institution of Great Britain, London, UK*)
   'Modelling of Defects in Minerals'
   'Interatomic Potentials'
9. M.Dove (*University of Cambridge, UK*)
   'Reverse Monte-Carlo methods'
10. M.Carpenter (*University of Cambridge, UK*)
    'Microscopic strain, macroscopic strain, thermodynamics and phase transitions'
11. C.Geiger (*Universitaet Kiel, Germany*)
    'Vibrational Properties & Thermodynamics of Silicates - Micro-macro relationships'
12. G.Artioli (*Universitá di Milano, Italy*)
    'Atomic displacement parameters from diffraction studies: the experimental evidence'

The school will provide plenty of opportunities for discussion with some of the best experts in the field, and the participants will be able to present their posters (which will be published in the journal 'Acta Mineralogica Petrographica' and also in a book of Abstracts). Budapest and the organisers of the school will also provide plenty of opportunities for sightseeing!

The Second Circular, registration form, and more detailed information can be found at the official Website of the School:

`http://slamdunk.geol.ucl.ac.uk/~artem/EMU-School.html.`

The registration (and payment) deadline is 15 JUNE. The decision of the Bursary Committe will become available on 16 JUNE.

The registration fees are as follows: 350 EURO before, and 400 EURO after June 15, 2002, which includes participation, accommodation (6 nights, double room with shower/bath); lecture notes (over 400 printed pages), programme and abstracts booklet; boat trip, refreshments in breaks; welcome party; farewell dinner. Accompanying persons' registration fee (EURO 310) covers accommodation (6 nights); boat trip, welcoming party and farewell dinner. A limited number of bursaries are available, with preference for participants from the poorer countries.

Please see the School's website or contact us (emu@ulixes.elte.hu; Carlo.Gramaccioli@unimi.it; a.oganov@ucl.ac.uk) for any enqueries.

As experience shows, each Summer School of the European Mineralogical Union is an unforgettable event. We look forward to meeting you and/or your students in Budapest.

Carlo Gramaccioli and Tamas Weiszburg

Organisers of the School

6.7 Summer School on Linear-scaling Ab-initio Molecular Modelling of Environmental Processes

Cambridge 15-17 July 2002

http://www.niees.ac.uk

Organised by Emilio Artacho and Martin Dove

This school will focus on linear-scaling DFT based on localised atomic orbitals. The school will include practical sessions using the SIESTA code. Lecturers will include Emilio Artacho, Julian Gale, Alberto Garcia, Javier Junquera and Jose Soler.

Find detailed information at the above web page.

The school is offered by the National Institute of Envirnomental eScience.

6.8 ChiPPS Workshop

3rd International Workshop on

Challenges in Predictive Process Simulation

Prague, Czech Republic, 13-17 Oct 2002
http://www.ihp-ffo.de/chipps/02/

`Diffusion-Growth-Defects-Fabrication-Devices-Ideas-Today-Future`
`--> from experiment and simulation to design and production <--`
`Problem-Constraints-Method-Mechanism-Model-Calibration-Solution`

Organized by IHP-microelectronics **Sponsored by Avant!**

ChiPPS is a series of meetings aimed to bring together experts from three distinct fields:

- fundamental materials science,
- development of process simulation tools,
- manufacture of microelectronic devices.

In particular, it serves as a bridge between those who study physical properties at the atomic scale and those who simulate technological processing steps at the macroscopic level.

Sample subjects of interest are:

- Diffusion in solids
- Carrier transport in nanostructures
- Deposition of dielectrics and metals
- Epitaxial growth of semiconductors
- Formation of silicide films
- Reliability of dielectrics and interconnects
- Integration of microelecronic and optoelectronic devices
- New materials for microelectronics
- New concepts for microelectronic devices

More information:	**www.ihp-ffo.de/chipps/02/**
Registration:	**www.ihp-ffo.de/chipps/02/register.html**
To receive regular posting:	contact *chipps@ihp-ffo.de*

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7 General Job Announcements

Postdoctoral Research Associate

CONDENSED MATTER AND MATERIALS PHYSICS GROUP
DEPARTMENT OF PHYSICS AND ASTRONOMY
UNIVERSITY COLLEGE LONDON, LONDON, UK

Applications are invited from theoretical physicists for Postdoctoral Research Associate positions in the CMMP group at the Department of Physics and Astronomy, University College London. The group is engaged into theoretical research and computer modelling and simulation of a wide spectrum of processes in condensed matter, ranging from behaviour of matter in the Earth's core to properties of nano-wires and modelling atomic manipulation using Scanning Probe Methods. Applications will be considered in the following two areas:

(1) Theory of defects in amorphous SiO2 for opto- and microelectronics applications. This project will focus on a theory of electronic structure and spectroscopic properties of defects responsible for fibre Bragg gratings and optical nonlinearity of GeO2-SiO2 glasses. The project will also contribute to our understanding of the mechanisms of breakdown of amorphous silica films in electronic devices. A PDRA is required to model silica glasses and to develop models of defects and defect processes in these materials responsible for Bragg grating formation and stability.

(2) Theory of defects and defect processes in high-K dielectric films on Si. This project will focus on theoretical studies of the structure, electronic and dielectric properties, and stability of oxide films on silicon. It should address the effect of structural defects, impurities and surface defects on the dielectric properties and performance of oxide films as gate dielectrics. A PDRA is required to model the structure of oxide films (such as ZrO2, HfO2 and their silicates) on silicon, and to develop models of defects and defect processes in these materials responsible for the electronic properties and degradation of these films.

Positions are available initially for two years with possible further extension. Persons appointed will be responsible to Dr Alexander Shluger and will collaborate with other members of CMMP. A PhD in a relevant theoretical field and research experience in theoretical modelling of solids using classical atomistic simulation and/or advanced quantum-mechanical methods is essential.

An appointment will be made at the Research Fellow level (Research Staff scale IA, 19,760 - 28,625 GBP, including London Allowance) depending on the background and experience of the candidate.

For further information please contact Dr Alexander Shluger (a.Shluger@ucl.ac.uk, + 44 (0)20 7679 1312); http://www.cmmp.ucl.ac.uk/)

Applications should include a CV and publication list, names and addresses of two referees and a covering letter summarising the candidate's research interests and experience. They should be sent to Dr Alexander Shluger by May 30, 2002.

Dr Alexander Shluger
Department of Physics and Astronomy
University College London
Gower Street, London WC1E 6BT, UK

tel. : 44 20 7679 1312
FAX: 44 20 7679 1360

JUNIOR PROFESSOR IN THEORETICAL PHYSICS
Technical University of Clausthal, Germany

The Technical University of Clausthal is currently establishing junior professorships with financial support from the German Federal Government and the Federal State of Lower Saxony. The Technical University of Clausthal is building up a tight-knit network of interdisciplinary research groups ranging from theoretical physics to materials engineering linking basic research to technology.

Therefore it performs an international search for a JUNIOR PROFESSOR IN THEORETICAL PHYSICS, preferably in one of the following research areas: (1) Light-matter interaction in structured materials (e.g. photonic crystals, nonlinear optic effects); (2) Dynamics of the microstructure of materials (grain boundaries and dislocation networks). For further information see http://www.pt.tu-clausthal.de/jp.shtml.

The position is expected to be filled in 2002. Prerequisites for appointment include a doctorate of outstanding quality dating back not more than five years, further scientific achievernents after completion of the doctorate and teaching abilities. The duties of a newly appointed junior professor at Technical University of Clausthal include independent research, teaching, continuing education and service to the community as part of the activities of an institute he or she will be affiliated with. The facilities provided should enable the successful applicant to procure external funding and to acquire qualifications for a professorial appointment. The initial appointment will not be bound to the current salary scale, the salary level being set to correspond to VergGr. lb BAT. lf the prerequisites pursuant to the public service and budgetary legislation are satisfied, the successful applicant will be appointed as a public servant on a temporary basis and designated junior professor, salary level Wl. The employment contract will initially be limited to three years, with a possibility of extension by a further three year period subject to evaluation. aluation.

The Technical University of Clausthal is committed to increasing the proportion of women among its staff and therefore strongly encourages women to apply. Preference will be given to severely handicapped persons with appropriate qualifications. Applications must be submitted to the Rector of the Technical University of Clausthal by **May 31, 2002**.

Address:

Technische Universitaet Clausthal
Rektorat
Adolph-Roemer-Strae 2A
D-38678 Clausthall-Zellerfeld, Germany

Postdoctoral Position(s)

Carnegie Mellon University and Oak Ridge National Laboratory

One or two postdoctoral positions in theoretical condensed matter physics are available at Carnegie Mellon University and/or Oak Ridge National Laboratory as part of a DARPA funded project studying metallic glass. We seek researchers who can develop and apply ab-initio electronic structure methods for aperiodic structures or who can apply statistical mechanics and computer simulation methods to model the structure and formation of metallic glass.

The positions are available immediately.

Applications will be accepted until the positions are filled. For further information, contact Don Nicholson(dmn@ornl.gov) or Michael Widom (widom@andrew.cmu.edu).

Postgraduate Studentship

"Simulating Biomineral Growth and Surface Order in Iron Oxides"

NMRC Ireland

NMRC Ireland http://www.nmrc.ie is a specialised ICT research centre in areas including nanofabrication, photonics and microelectronics. Applications are invited for a postgraduate studentship in computational modelling at NMRC to investigate the surface science of iron oxides as part of the IRCSET-funded 'FeOx' project.

Materials properties may be finely tuned if growth at the atomic scale is controlled, but fundamental knowledge about growth mechanisms is scant. This project focusses on perhaps the most ancient case of controlled growth: the biomineralisation of magnetite. To study the complex patterns of spin and valence ordering in a range of cubic iron oxides (including magnetite), the atomic and electronic structure will be calculated by Density Functional Theory using slab and cluster models. By identifying the manner in which iron oxide surfaces reconstruct, oxidation states involved and the effect of ambient dielectric, the mechanism of oxide growth can be determined.

NMRC is located in the vibrant city of Cork, near the stunning landscapes of Ireland's southern coast. Postgraduate students at NMRC receive an annual stipend of over EUR 15000 and register at University College Cork for Masters or Ph.D http://www.ucc.ie

The studentship is available from October 2002. Candidates of any nationality with a strong primary degree in chemistry, physics, computational or materials science or a related discipline are welcomed. An interest in such areas as electronic structure theory, computational modelling, surface physics or bio-inorganic chemistry is advantageous.

For informal inquiries please contact mailto: Simon.Elliott@nmrc.ucc.ie, Tel: +353-21-490 4392;
NMRC, Lee Maltings, Prospect Row, Cork, Ireland; and for more information see http://www.nmrc.ie/feox.

Research Studentship

”First Principles Study of Colossal Magnetic Resistance in Magnetic Oxides”

Department of Physics and Astronomy Sheffield University and Daresbury Laboratory, UK

The mixed oxides of manganese have a large range of properties that are manifest as the doping concentration is changed. The most well known of these is the colossal magnetoresistance that appears near to the ferromagnetic phase transition. However, these materials are what is known as 'half metallic ferromagnets' which means that the Fermi level lies in the density of states for one spin band (as for a metal) and in a band gap for the other spin component (as for a semiconductor). This means that the materials are extremely promising for use in spin injection devices where a current is carried entirely by electrons of one spin. Unfortunately the surfaces of the material may have imperfections leading to a rapid loss of spin purity as the temperature is raised. The research project is to calculate the electronic properties of the manganites at surfaces and grain boundaries. These calcuations will be very important as they will indicate if the effects that are seen are actually intrinsic to the manganite surfaces or if there are ways to overcome these problems. The work will build on the work of the last student to work in this collaboration who developed methods to study the charge, orbital and spin ordering in manganites from first principles.

The studentship is available with joint supervision from Professor G. A. Gehring (Sheffield) and Professor W. M. Temmerman (Daresbury). The student would spend the first year based in Sheffield and the second two years based in Daresbury. Throughout the project there would be regular meetings of the student with both supervisors.

This is an established collaboration between Professors Gehring and Temmerman which has had a succession of students (4) all of whom have completed their PhD's satisfactorily and on time.

For further information please contact: Professor Gillian A. Gehring (g.gehring@sheffield.ac.uk) or Professor Walter M. Temmerman (w.m.temmerman@dl.ac.uk).

Application forms from: Miss K Low (k.low@sheffield.ac.uk), Department of Physics & Astronomy, University of Sheffield, Hicks Building, Sheffield, S3 7RH, UK. Tel: +44 (0)114 222 3519.

Postdoctoral Position

"MULTI-SCALE CLASSICAL AND QUANTUM SIMULATIONS TO STUDY ENZYME FUNCTION"

Department of Physics, Rensselaer Polytechnic Institute
Troy, NY

An immediate opening is available to develop multi-scale classical and quantum simulations as applied to an exciting biological problem. The research will involve molecular level studies of a self-splicing mechanism of proteins known as inteins that have novel applications in biotechnology such as in bioseparations, sensors and drug delivery. Inteins are known to interrupt other proteins and are removed by a self-splicing process (Paulus, 2000). The goal of the research is to unravel the mechanism of intein cleavage using a novel two-prong theoretical approach involving classical molecular dynamics and quantum ab-initio calculations. Currently, there is no understanding why increased cleavage occurs at higher temperature (20 versus 37 degrees C) and/or at lower pH values (pH 8.0 versus 6.5) (Wood et al., 2000). Previous work in our labs using saturation mutagenesis has shown that cleavage rates can be substantially increased with relatively minor amino acid substitutions (Wood et al., 1999). The computational work for which a post doc is being sought will be complemented by site-directed mutagenesis work and will help explain the pH and temperature dependence of the cleavage reaction. Candidates with a strong background in the applications of molecular dynamics and/or quantum dynamics methods are encouraged to apply. Appointment is for one year with the possibility of extension dependent on performance. FAX or E-mail curriculum vitae and names of three references with telephone numbers and e-mail addresses to:

Professor Saroj Nayak
Department of Physics
Rensselaer Polytechnic Institute
Troy, NY 12180-3590
E-mail: nayaks@rpi.edu

or

Professor Shekhar Garde
Isermann Department of Chemical Engineering
Rensselaer Polytechnic Institute
110 8th Street, Troy NY 12180
gardes@rpi.edu

Relevant publications:

1. Paulus, H. Protein splicing and related forms of protein autoprocessing, Ann Rev. (2000) 447-496.

2. Wood, D. W., Wu, W., Belfort, G., Derbyshire, V. and Belfort, M. A genetic system yields self-cleaving inteins for bioseparations. Nature Biotech. (1999) 17, 889-892.

3. Wood, D., Derbyshire, V. Wu, W., Chartrain, M., Belfort, M., and Belfort, G. Optimized Single-Step Affinity Purification with a Self-Cleaving Intein Applied to a Human Fibroblast Growth Factor. Biotechnology Progress (2000) 16, 1055-1063.

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PhD Studentship in Manchester, UK
Project: Oilfield Barite Scale Formation and Inhibition: Designing Solutions to a Costly Problem

A NERC-funded Industrial CASE studentship is available from October 2002 to study the inhibition of barite scale using both experimental (e.g. STM and TEM) and theoretical (both first-principles and empirical) techniques. The project is motivated by the enormous problems encountered by the oil industry in dealing with scale in oil pipelines and the student will spend some time working at BP. BP's support also includes a generous supplement to the maintenance grant so that the total stipend is expected to be 11350 GBP p.a.

The project complements ongoing research into the growth of barite (BaSO4) in realistic oil pipeline conditions. It aims to determine the dominant morphologies of barite scale, the relationships between the morphology, crystallography and chemistry of barite and the effects of commercial scale inhibitors. It offers opportunities to work in a truly multi-disciplinary setting on start-of-the-art equipment as well as contact with industry and access to real oilfield data. Training will be provided in experimental, analytical and computational techniques. The supervisors are Dr M. Warren, Dr M. Farquhar and Prof D.Vaughan at the Williamson Research Centre and Dept of Earth Sciences, University of Manchester, and Dr I. Collins from BP Exploration.

Applicants should have or be expecting a 1st or 2.1 degree (or equivalent) in physics, chemistry or a geoscience subject. Full NERC funding (fees + stipend as above) is only available to UK students; other EU students may be eligible for fees-only awards. Applications should be made via the department: see below for contact details or use the online form available via our website. Informal enquiries in advance of an application can be made to Dr M. Warren, m.c.warren@man.ac.uk or +44-(0)161 275 3808. Applications should be made as soon as possible and definitely before the end of July 2002.

The Department was awarded RAE grade 5 in 2001, and has 28 permanent academic staff, 28 research staff and 27 support staff. The recent establishment of the interdisciplinary Williamson Research Centre for Molecular Environmental Science, housed within the department, brought over 3M GBP of government funding for laboratory refurbishment and major new items of equipment.

More information is available from the department's website, http://www.man.ac.uk/Geology/ or by contacting the Postgraduate Secretary:

The Postgraduate Secretary,
Department of Earth Sciences, The University of Manchester,
Oxford Road, Manchester, M13 9PL, UK
Telephone: +44-(0)161 275 0801, Email: adminw@fs1.ge.man.ac.uk

PostDoc in Computational Magnetism
Trinity College Dublin

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

The fellowship, tenable for up to 3 years, will commence on or after the 1st October 2002 with an annual salary ranging between 26.702 and 36.178 Euros, depending on the experience of the candidate. The Physics Department at Trinity College Dublin has a long and distinguished history of research. Currently the department is host of the prestigious first phase of Science Foundation of Ireland Nanotechnology projects, attracting world class researchers and establishing internationally competitive facilities. Finally it is worth mentioning that Dublin is a vital, young European capital, and a very pleasant place to live.

Candidates for this fellowship are invited to send a CV, a brief description of their research interests and their experience, and the full contact address of two referees by post or e-mail to:

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

Information about the research activity may be found at:
http://www.tcd.ie/Physics/People/Stefano.Sanvito/ .
Further particulars regarding the Fellowship may also be obtained from Dr. Sanvito.

PhD Position in Computational Magnetism
Trinity College Dublin

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

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

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Dr. Stefano Sanvito
Department of Physics
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8 Abstracts

Exchange interactions in NiO and at the NiO(100) surface

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Abstract

The electronic and magnetic structure of bulk NiO and the NiO(100) surface is calculated using density functional theory (DFT) in the local spin density (LSD) approximation including self-interaction corrections (SIC). We calculate the exchange coupling constants in bulk NiO and at the NiO(100) surface and show that in the case of bulk they agree better with experiment than the standard DFT calculations in the LSD approximation. We develop a model for the exchange interactions at the NiO(100) surface and discuss how they change from the surface to bulk.

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Quenching of majority-channel quasiparticle excitations in cobalt

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Abstract

The low-energy electronic excitations in cobalt are studied using a theoretical method that includes both a realistic description of the band structure and an accurate treatment of many-body electron-electron interactions. Angle-resolved photoemission spectra were measured on a thick film of hexagonal close-packed Co on Cu(111); they agree well with calculated spectral functions. Due to many-body effects no sharp quasiparticle peaks exist for binding energies larger than 2 eV and in this energy region the spectrum is essentially incoherent. This is due to the heavy mixing of many excited configurations occurring because of the high density of holes in the valence band. The many-body corrections turn out to be much stronger in the majority-spin channel and drastically affect the spin polarization of the spectra.

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XRMS study of the magnetic coupling in Co/Pt nanolines and its evolution under magnetic field

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Abstract

Periodic arrays of silicon nanolines, covered by a Co/Pt multilayer, with perpendicular magnetization, have been studied by soft X-ray Resonant Magnetic Scattering (XRMS), at the Co L_3 edge. At the resonance, magnetic signals appear both on top of the structural diffraction peaks, characteristic of the grating, and between these peaks. These superstructure satellites reveal an antiferromagnetic order, generated by the interline dipolar coupling. Their intensities are strongly sensitive to the magnetic history, and can be enhanced through specific demagnetization processes. By applying an in-situ magnetic field, the evolution of the magnetic signal has been monitored through the entire hysteresis loop. The magnetic contribution of the structural superlattice peaks can be quantified by their asymmetry ratio, whose angular variation stems from the scattering factor. The change of the purely magnetic satellites with the magnetic field is completely reproducible and characterizes the modifications of the magnetic configuration during the reversal process. A model of Ising macrospins, from which the distribution of the magnetic reversal fields can be deduced, is shown to be in agreement with the measured results.

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Quantum Monte Carlo calculations of H_2 dissociation on Si(001)

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Abstract

We present quantum Monte Carlo calculations for various reaction pathways of H_2 with Si(001), using large model clusters of the surface. We obtain reaction energies and energy barriers noticeably higher than those from approximate exchange-correlation functionals. In improvement over previous studies, our adsorption barriers closely agree with experimental data. For desorption, the calculations give barriers for conventional pathways in excess of the presently accepted experimental value, and pinpoint the role of coverage effects and desorption from steps.

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Atomistic Simulations of Processes at Surfaces

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Abstract

In this contribution, a review of the methodology for atomistic modeling of surface processes is given. The focus will be on the physical background of the methods used, their range of applicability, and their strengths and weaknesses for addressing specific problems. However, a few examples of selected applications will be presented as well. Some room will be given to the discussion of methods to calculate total energies and forces, which form the basis for any kind of process simulation. Here I shall give an overview ranging from the computationally least demanding methods applying analytical potentials to more involved techniques that account for the quantum-mechanical nature of chemical bonding. This includes the semi-empirical tight-binding method, as well as first-principles calculations. Density-functional theory will be introduced and described in some detail, and a brief discussion of the benefits of quantum-chemical *ab initio* methods, such as Hartree-Fock and the configuration-interaction method, is given. When applying simulation techniques for processes at the atomic level, we have to distinguish between activated and non-activated molecular processes. These two types of processes require different simulation tools. While the well-documented molecular dynamics method is the method of choice for modeling non-activated processes, methods for treating activated processes are still less wide-spread. Therefore I shall describe in some detail the foundations of the kinetic Monte Carlo approach and its combination with first-principles calculations that opens up the capability to perform predictive simulations for systems in which activated processes play a dominant role. As an example, simulations of island nucleation in molecular beam epitaxy of GaAs will be presented. Finally, I will conclude by discussing prospects of future modeling of processes at surfaces that could bring us closer to the goal of predictive process simulations.

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Magneto-optical properties of ultra-thin surface layer systems

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Abstract

A first-principle description of the magneto-optical Kerr effect (MOKE) of ultra-thin surface layer systems is presented, that is based on the concept of the non-local layer-resolved optical conductivity and the corresponding solution of the Maxwell equations. This powerful approach allowed a detailed investigation of the system Au(001)/nFe/mAu that shows pronounced quantum confinement effects. In particular insight into the spatial origin of magneto-optical properties was obtained and the reliability of simplified approaches could be checked that way for this important prototype surface layer system.

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9 SCIENTIFIC HIGHLIGHT OF THE MONTH

Half-ferromagnetism and Slater-Pauling behavior in the Heusler alloys

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Abstract

The development of magnetoelectronics has increased the interest in materials which can enhance the performance of spin-dependent devices. Such materials are the so-called half-metals which present a gap in the minority band resulting in 100% spin-polarization at the Fermi level. A significant number of the intermetallic Heusler alloys have been predicted to be half-metals. In this contribution I present a complete study of both the bulk and surface properties of such Heusler alloys including both the families of the so-called half-Heusler alloys like NiMnSb and of the full-Heusler alloys like Co_2MnGe. Based on the *ab-initio* results for these compounds I discuss the origin of the gap which is fundamental for the understanding of their electronic and magnetic properties. I show that for both families of compounds the total spin magnetic moment M_t scales with the number of valence electron Z_t, such that $M_t = Z_t - 18$ for the half-Heusler and $M_t = Z_t - 24$ for the full-Heusler alloys, thus opening the way to engineer new half-ferromagnetic Heusler alloys with the desired magnetic properties. Although the surfaces loose in-general the half-ferromagnetic character and exhibit a small degree of spin-polarization, I show that in the case of compounds containing Cr, the large enhancement of the Cr moments at the surface reduces the effect of the surface states and leads to a very high spin-polarization of the surfaces, *e.g* 84% for the CrAl-terminated $Co_2CrAl(001)$ surface or even 100% for the Cr-terminated CrAs(001) surface, so that these compounds might be promising for spindependent devices.

[⋆] Young researcher within the RT-Network "Computational Magnetoelectronics". Work was performed in collaboration with Nikos Papanikolaou, University of Halle-Wittenberg, and Peter H. Dederichs, Forschungszentrum Jülich.

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1. Introduction

Heusler alloys [1] have attracted during the last century a great interest due to the possibility to study in the same family of alloys a series of interesting diverse magnetic phenomena like itinerant and localized magnetism, antiferromagnetism, helimagnetism, Pauli paramagnetism or heavy-fermionic behavior [2, 3, 4, 5]. The first Heusler alloys studied were crystallizing in the $L2_1$ structure which consists of 4 fcc sublattices. Afterwards, it was discovered that it is possible to leave one of the four sublattices unoccupied ($C1_b$ structure). The latter compounds are often called half-Heusler alloys, while the $L2_1$ compounds are referred to as full-Heusler alloys. In a pioneering theory paper in 1983 de Groot and his collaborators [6] showed that one of the half-Heusler compounds, NiMnSb, is a half-ferromagnet, i.e. the minority band is semiconducting with a gap at the Fermi level E_F, leading to 100% spin polarization at E_F. Such half-ferromagnets can be considered as hybrids between metals and semiconductors. Recently the rapid development of magnetoelectronics intensified the interest on such materials since the efficiency of any spindependent device scales with the spin-polarization. Adding the spin degree of freedom to the conventional electronic devices has several advantages like nonvolatility, increased data processing speed, decreased electric power consumption and increased integration densities [7]. The current advances in new materials are promising for engineering new spintronic devices in the near future [7]. Other known half-ferromagnetic materials are *e.g.* CrO_2 [8], $La_{0.7}Sr_{0.3}MnO_3$ [8], the diluted magnetic semiconductors like (In,Mn)As [9] and very recently also CrAs in the zinc-blende structure was proposed to be a half-ferromagnet [10]. Although thin films of CrO_2 and $La_{0.7}Sr_{0.3}MnO_3$ have been verified to present practically 100% spin-polarization at the Fermi level at low temperatures [8, 11], the Heusler alloys remain attractive for technical applications like spin-injection devices [12], spin-filters [13], tunnel junctions [14], or GMR devices [15] due to their relatively high Curie temperature compared to these compounds [2].

The half-ferromagnetic character of NiMnSb in single crystals has been well-established experimentally. Infrared absorption [16] and spin-polarized positron-annihilation [17] gave a spin-polarization of ~100% at the Fermi level. Recently it has also become possible to grow high quality films of Heusler alloys, and it is mainly NiMnSb that has attracted the attention [18]. Unfortunately these films were found not to be half-ferromagnetic [8, 19, 20, 21]; a maximum value of 58% for the spin-polarization of NiMnSb was obtained by Soulen *et al.* [8]. These polarization values are consistent with a small perpendicular magnetoresistance measured for NiMnSb in a spin-valve structure [22], a superconducting tunnel junction [14] and a tunnel magnetoresistive junction [23]. Ristoiu *et al.* showed that during the growth of the NiMnSb thin films, Sb and then Mn atoms segregate to the surface, which is far from being perfect, thus decreasing the obtained spin-polarization [24]. But when they removed the excess of Sb by flash annealing, they managed to get a nearly stoichiometric ordered alloy surface being terminated by a MnSb layer, which presented a spin-polarization of about 67±9% at room temperature [24]. The temperature dependence of the spin moments for such a film was studied by Borca *et al.* [25].

Several groups have verified the half-ferromagnetic character of bulk NiMnSb using first-principles calculations [26, 27]. Larson *et al.* have shown that the actual structure of NiMnSb is the most stable with respect to an interchange of the atoms [28] and Orgassa *et al.* showed that a few percent of disorder induce states within the gap but do not destroy the half-metallicity [29]. Recently, Wijs and de Groot have shown by first-principle calculations that NiMnSb surfaces do not present 100% spin-polarization and they proposed that at some interfaces it is possible to restore the half-ferromagnetic character of NiMnSb [30]. Also recently, Jenkins and King studied by a pseudopotential technique the MnSb terminated (001) surface of NiMnSb and showed that there are two surface states at the Fermi level, which are well localized at the surface layer [31] and they persist even when the MnSb surface is covered by a Sb overlayer [32].

Webster and Ziebeck [33] and Suits [34] were the first to synthesize full-Heusler alloys containing Co and Rh, respectively. Kübler *et al.* studied the mechanisms stabilizing the ferro- or the antiferromagnetism in these compounds [35]. Ishida and collaborators have proposed that the compounds of the type Co_2MnZ, where Z stands for Si and Ge, are half-ferromagnets [36, 37]. Also the Heusler alloys of the type Fe_2MnZ have been proposed to show half-ferromagnetism [38]. But Brown *et al.* [39] using polarized neutron diffraction measurements have shown that there is a finite very small spin-down density of states (DOS) at the Fermi level instead of an absolute gap in agreement with the *ab-initio* calculations of Kübler *et al.* for the Co_2MnAl and Co_2MnSn compounds [35]. Recently, Ambrose *et al.* managed to grow a Co_2MnGe thin film on a GaAs(001) substrate by molecular beam epitaxy [40], and there also exist first-principles calculations for the (001) surface of such an alloy [41]. Finally, Geiersbach and collaborators have grown (110) thin films of Co_2MnSi, Co_2MnGe and Co_2MnSn using a metallic seed on top of a MgO(001) substrate [42].

In this contribution, I present a complete study of both the bulk and surface properties of the Heusler alloys. In total I have identified about thirty half-metallic compounds. Analyzing the *ab-initio* results using the group-theory and simple models I explain the origin of the gap in both the half- and full-Heusler alloys, which is fundamental for understanding their electronic and magnetic properties. For both families of compounds the total spin magnetic moment scales with the number of valence electron, thus opening the way to engineer new half-ferromagnetic Heusler alloys with the desired magnetic properties. Although in general the surfaces loose the half-ferromagnetic character and show only a small degree of spin-polarization, I show that in the case of compounds containing Cr, the very large Cr moments at the surface reduce the importance of the surface states and the spin-polarization of such surfaces is very high, *e.g* 84% for the CrAl-terminated $Co_2CrAl(001)$ or even 100% for the Cr-terminated CrAs(001) surface. Thus these compounds might be promising for spindependent devices.

In Section 2 I present the details of my calculations and in section 3 the electronic and magnetic properties of the XMnSb (X=Ni,Co,Rh,Pd,Ir or Pt) and Co_2MnZ (Z=Al,Si,Ga,Ge or Sn) compounds. In Section 4, I investigate the origin of the gap and the Slater-Pauling behavior. In Sections 5 and 6 I study the surface properties of the Heusler alloys and of CrAs, respectively. Finally in Section 7 I conclude and summarize my results. For a more extended presentation of the results presented in this manuscript, the reader is referred to the papers in Ref. [43].

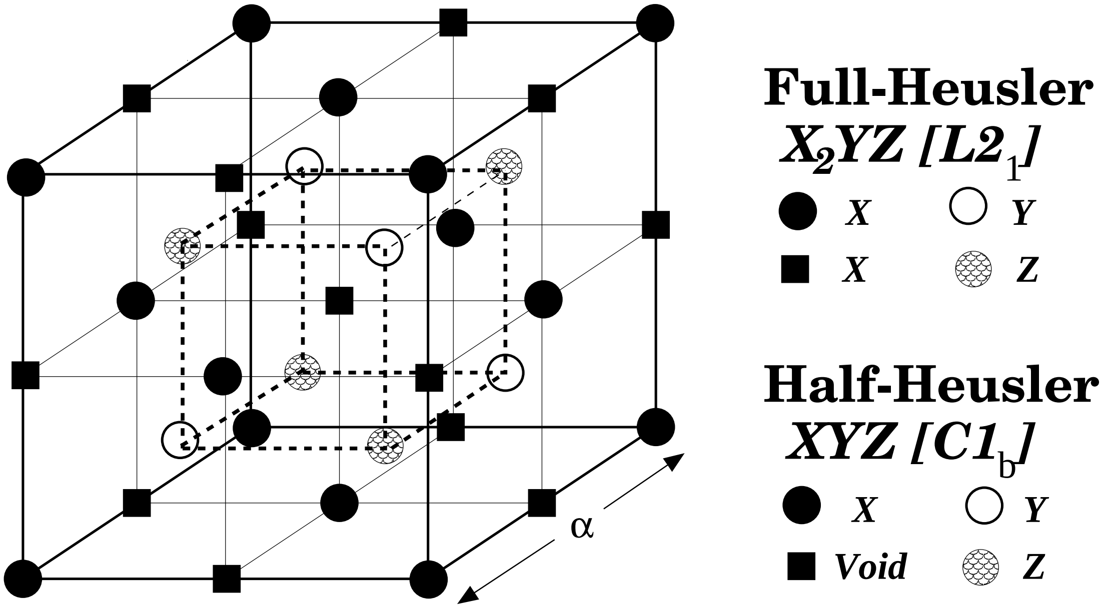

Figure 1. Schematic representation of the $C1_b$ and $L2_1$ structures. The lattice consists of 4 fcc sublattices. The unit cell is that of a fcc lattice with four atoms as basis, *e.g.* CoMnSb: Co at (0 0 0), Mn at ($\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4}$), a vacant site at ($\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$) and Sb at ($\frac{3}{4}\,\frac{3}{4}\,\frac{3}{4}$) in Wyckoff coordinates. In the case of the full Heusler alloys also the vacant site is occupied by a Co atom.

2. Computational Details

To perform the calculations, I used the Vosko, Wilk and Nusair parameterization [44] for the local density approximation (LDA) to the exchange-correlation potential [45] to solve the Kohn-Sham equations within the full-potential screened Korringa-Kohn-Rostoker (FSKKR) method [46, 47]. The full-potential is implemented by using a Voronoi construction of Wigner-Seitz polyhedra that fill the space as described in Ref. [47]. A repulsive muffin-tin potential (4 Ry high) is used as reference system to screen the free-space long-range structure constants into exponentially decaying ones [48]. For the screening I took for all the compounds interactions up to the sixth neighbors into account leading to a tight-binding (TB) cluster of 65 neighbors around each atom. To calculate the charge density, I integrated along a contour on the complex energy plane, which extends from the bottom of the band up to the Fermi level [49]. Due to the smooth behavior of the Green's functions for complex energies, only few energy points are needed; in my calculations I used 42 energy points. For the Brillouin zone (BZ) integration, special points are used as proposed by Monkhorst and Pack [50]. Only few tens of **k** are needed to sample the BZ for the complex energies, except for the energies close to the real axis near the Fermi level for which a considerably larger number of **k**-points is needed. I have used a 30×30×30 **k**-space grid in the full BZ to perform the integrations in the case of the bulk calculations and a two-dimensional 30×30 $\mathbf{q}_{||}$-space grid in the case of the surfaces. In addition I used a cut off of ℓ_{max}=6 for the multipole expansion of the charge density and the potential and a cut off of ℓ_{max}=3 for the wavefuctions. Finally in my calculations the core electrons are allowed to relax during the self-consistency. In all the calculations I have used the experimental lattice constants [2].

To simulate the surfaces I have used a slab with 15 metal layers embedded in half-infinite vacuum from each side. Such a slab has two equivalent surfaces avoiding the creation of slab-dipoles. This slab thickness is sufficiently large so that the layers in the middle exhibit bulk properties; they show a spin-down gap of the same width as in the bulk and the same relative position of the Fermi level and finally the magnetic moments differ less than $0.01\mu_B$ from the bulk values.

In Fig. 1, I show the $C1_b$ and $L2_1$ structures adopted by the half- and full-Heusler alloys, respectively. Both structures consist of four fcc sublattices. A half-Heusler compound has the general formula XYZ, where X is a high-valent transition metal atom, Y a lower-valent transition metal atom and Z a *sp* atom. The unit cell is that of a fcc lattice with four atoms as basis: X at (0 0 0), Y at $(\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4})$, a void at $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$ and the Z atom at $(\frac{3}{4}\,\frac{3}{4}\,\frac{3}{4})$ in Wyckoff coordinates. In the case of a full Heusler alloy also the void site is occupied by a X-type atom. Note that in the case of the (001) surfaces there are two different possible terminations. One contains the Y and Z type atoms while the other one contains the X atoms (and the vacant site in the case of the half-Heusler compounds).

I should also mention that the structure of the Heusler alloys is similar to the zinc-blende structure adopted by a large number of semiconductors, like GaAs, ZnSe, InAs etc, which can also be considered of consisting of four fcc sublattices. In the case of GaAs the black spheres are occupied by Ga atoms and the empty spheres by As atoms, while the other two sites are vacant. This close structural similarity should make the Heusler alloys compatible with the existing semiconductor technology and thus very attractive for industrial applications.

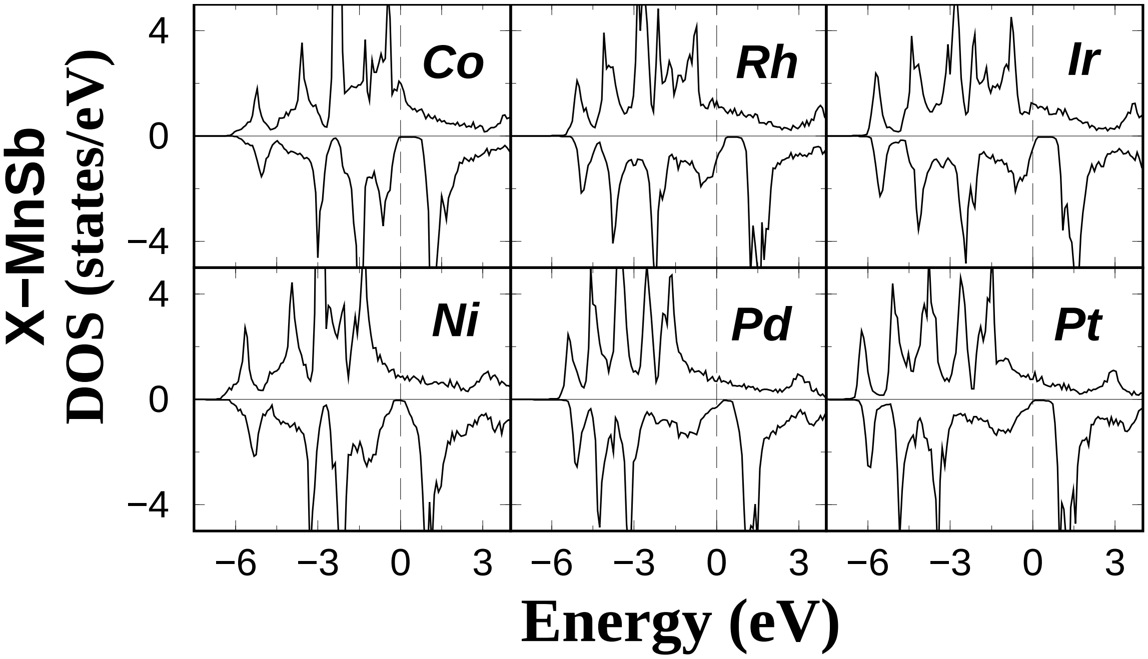

Figure 2. Spin-projected density of states for the XMnSb half-Heusler alloys. They all posses a spin-down gap but only in Co-, Ni- and Pt- based alloys the Fermi level (zero at the energy axis) falls inside the gap.

3. Electronic and Magnetic Properties

3.1 Half-Heusler alloys: X-MnSb with X= Co, Ni, Rh, Ir, Pd and Pt

Firstly I calculated the electronic structure of the half-Heusler alloys of the type XMnSb, with X being an element of the Co or Ni columns in the periodic table. These compounds are known experimentally to be ferromagnets with high Curie temperatures ranging between 500 K and 700 K for the Co, Ni, Pd and Pt compounds, while the Curie temperatures of the Ir and Rh compounds are around room temperature.[2] These compounds are known to exhibit a small disorder [2], with the exception of CoMnSb [51]. In Fig. 2 I present the spin-projected total density of states (DOS) for all the six compounds. I remark that all six compounds present a gap, which is wider in the compounds containing Co, Rh or Ir than in Ni, Pd or Pt. Sb p states occupy the lowest part of the DOS shown in the figure, while the Sb s states are located $\sim$12 eV below the Fermi level. For the Ni compound the Fermi level is at the middle of the gap and for PtMnSb at the left edge of the gap in agreement with previous full-potential linear muffin-tin orbitals method (FPLMTO) calculations on these compounds [26]. The gap in the minority NiMnSb band is about 0.5 eV wide in good agreement with the experiment of Kirillova and collaborators [16], who analyzing their infrared spectra estimated a gap width of $\sim$0.4 eV. In the case of CoMnSb the gap is considerably larger ($\sim$1 eV) than in the previous two compounds and the Fermi level is located at the left edge of the spin-down gap. CoMnSb has been studied theoretically by Kübler using the augmented spherical waves (ASW) method. He found a DOS similar to mine, with a large gap of comparable width and the Fermi level was also located at the left edge of the spin-minority gap [52]. For the other three compounds the Fermi level is located below the gap, although in the case of PdMnSb and IrMnSb it is very near the edge of the gap.

The DOS of the different systems are mainly characterized by the large exchange-splitting of the Mn d states which is around 3 eV in all cases (this is clearly seen in the atom-projected DOS of NiMnSb in Fig. 4). This large exchange splitting leads to large localized spin moments at the Mn site; the existence of the localized moments has been verified also experimentally [53]. The localization comes from the fact that although d electrons of Mn are itinerant, the spin-down electrons are almost excluded from the Mn site. In Table 1 I present the spin magnetic moments at the different sites for all the compounds under study. Here I should mention that in order to calculate the moments I integrate the spin-projected charge density inside every Wigner-Seitz polyhedron. In my calculations these polyhedra were the same for every atom. Overall the calculated moments for the Ni, Pd and Pt compounds are in very good agreement with previous *ab-initio* results [26, 27]. Experimental values for the spin-moment at the Mn site can be deduced from the experiments of Kimura *et al.* [54] by applying the sum rules to their x-ray magnetic circular dichroism spectra and the extracted moments agree nicely with my results; they found a Mn spin moment of 3.85 μ_B for NiMnSb, 3.95 μ_B for PdMnSb and 4.02 μ_B for PtMnSb. In the case of the Co-, Rh-, and IrMnSb compounds the spin magnetic moment of the X atom is antiparallel to the Mn localized moment and the Mn moment is generally about 0.5 μ_B smaller than in the Ni, Pd and Pt compounds. The Sb atom is here again antiferromagnetically coupled to the Mn atom.

Table 1. Calculated spin magnetic moments in μ_B using the experimental lattice constants (see Ref. [2]) for the XMnSb compounds.

$m^{spin}(\mu_B)$	X	Mn	Sb	Void	Total
NiMnSb	0.264	3.705	-0.060	0.052	3.960
PdMnSb	0.080	4.010	-0.110	0.037	4.017
PtMnSb	0.092	3.889	-0.081	0.039	3.938
CoMnSb	-0.132	3.176	-0.098	0.011	2.956
RhMnSb	-0.134	3.565	-0.144	<0.001	3.287
IrMnSb	-0.192	3.332	-0.114	-0.003	3.022
FeMnSb	-0.702	2.715	-0.053	0.019	1.979

The total magnetic moment in μ_B is just the difference between the number of spin-up occupied states and the spin-down occupied states. In the half-ferromagnetic compounds all spin-down states of the valence band are occupied and thus their total number is, as in a semiconductor, an integer and the total magnetic moment is also an integer since the total valence charge is an integer. A detailed discussion of the relation between the total moment and the number of electrons will be given in Section 4. Here I notice only that the local moment per unit cell as given in Table 1 is close to 4 μ_B in the case of NiMnSb, PdMnSb and PtMnSb, which is in agreement with the half-ferromagnetic character (or nearly half-ferromagnetic character in the case of PdMnSb) observed in Fig. 2. Note that due to problems with the ℓ_{max} cutoff the KKR method can only give the correct integer number 4, if Lloyd's formula has been used in the evaluation of the integrated density of states, which is not the case in the present calculations. I also find that the local moment of Mn is not far away from the 4 μ_B although there are significant (positive) contributions from the X-atoms and a negative contribution from the Sb atom. In contrast to this I find that for the half-metallic CoMnSb and IrMnSb compounds the total moment is about 3 μ_B. Also the local moment of Mn is reduced, but only by about 0.5 μ_B. The reduction of the total moment to 3 μ_B is therefore accompanied by negative Co and Ir spin moments, *i.e* these atoms couple antiferromagnetically to the Mn moments. The hybridization between Co and Mn is considerably larger than between Ni and Mn. Therefore the minority valence band of CoMnSb has a larger Mn admixture than the one of NiMnSb whereas the minority conduction band of CoMnSb has a larger Co admixture than the Ni admixture in the NiMnSb conduction band, while the populations of the majority bands are barely changed. As a consequence, the Mn moment is reduced by the increasing hybridization, while the Co moment becomes negative, resulting finally in a reduction of the total moment from 4 to 3 μ_B. Here I should also note that further substitution of Fe for Co leads also to a half-ferromagnetic alloy with a total spin magnetic moment of 2 μ_B as has been already shown by de Groot *et al.* in Ref. [55] and by my calculations in Table 1. Finally, in the case of RhMnSb the Fermi level is considerably below the gap and thus a part of the spin-down states are unoccupied leading to a total spin magnetic moment larger than the 3 μ_B of CoMnSb and IrMnSb.

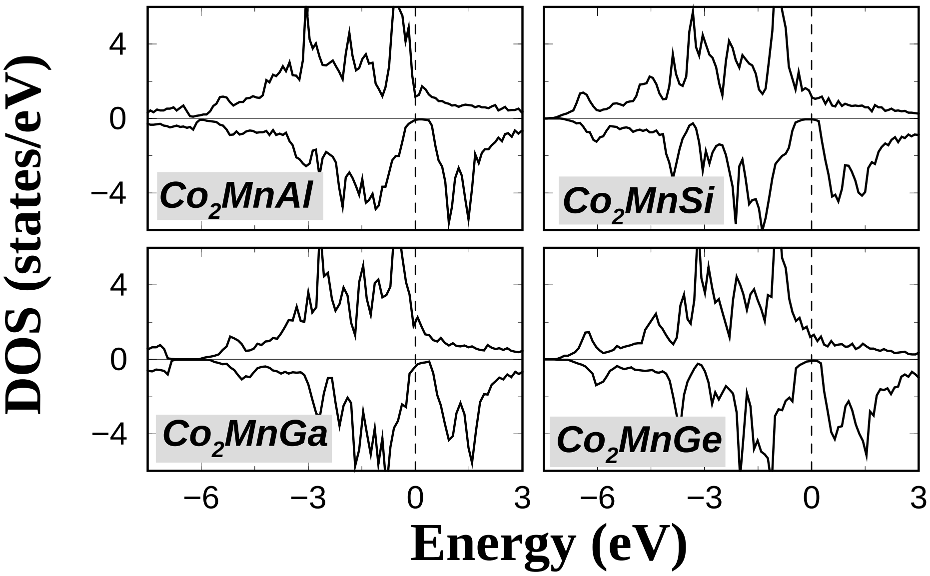

Figure 3. Calculated spin-projected DOS for the Co_2MnZ compounds, where Z stands for Al, Ga, Si and Ge. They all posses a finite very small spin-down DOS around the Fermi level.

3.2 Full-Heusler alloys: Co_2MnZ with Z= Al, Si, Ga, Ge and Sn

The second family of Heusler alloys, which I will discuss, are the full-Heusler compounds containing Co and Mn, as these are the full-Heusler alloys that have attracted most of the attention. They are all strong ferromagnets with high Curie temperatures (above 600 K) and except the Co_2MnAl they show very little disorder [2]. They adopt the $L2_1$ structure, which I present in Fig. 1. Each Mn or *sp* atom has eight Co atoms as first neighbors sitting in an octahedral symmetry position, while each Co has four Mn and four *sp* atoms as first neighbors and thus the symmetry of the crystal is reduced to the tetrahedral one. The Co atoms occupying the two different sublattices are chemically equivalent as the environment of the one sublattice is the same as the environment of the second one but rotated by 90^o. The occupancy of two fcc sublattices by Co (or in general by X) atoms distinguish the full-Heusler alloys with the $L2_1$ structure from the half-Heusler compounds with the $C1_b$ structure, like *e.g.* CoMnSb, where only one sublattice is occupied by Co atoms and the other one is empty. Although in the $L2_1$ structure, the Co atoms are sitting on second neighbor positions, their interaction is important to explain the magnetic properties of these compounds as I will show in the next section. In Fig. 3 I have gathered the spin-resolved total density of states (DOS) for the Co_2MnAl, Co_2MnGa, Co_2MnSi and Co_2MnGe compounds calculated using the FSKKR. Firstly as shown by photoemission experiments by Brown *et al.* in the case of Co_2MnSn [56] and verified by my calculations, the valence band extends 5 eV below the Fermi level and the spin-up DOS shows a large peak just below the Fermi level for these compounds. Although Ishida *et al.* [36] predicted them to be half-ferromagnets with small spin-down gaps ranging from 0.1 to 0.3 eV depending on the material, within my calculations I find that the Fermi level falls within a region of very small spin-down DOS for all these compounds. Our results agree with the calculations of Kübler *et al.* [35] who studied the Co_2MnAl and Co_2MnSn compounds using the Augmented Spherical Wave (ASW) method and found also a very small spin-down DOS at the Fermi level and not a real gap. The reason of this pseudogap can be found in Fig. 5 where I have drawn the band structure for the minority electrons in the case of the Co_2MnGe compound. I see that the Fermi level touches the highest occupied bands at the Γ point and the lowest unoccupied bands at the K and X points and thus the indirect gap found in the half-Heusler alloys [6] is practically destroyed in these materials but there is still a reasonably large direct gap at the K and X points. However I should mention that if I considerably enlarge the figure with the band structure, it can be seen that the bands do not really touch the Fermi level but there is a very small indirect gap of the order of 0.001 eV and thus the minimum of the minority unoccupied bands at L, K and X and the maximum of the occupied bands at the Γ point are not degenerated.

In the case of the half-Heusler alloys like NiMnSb the Mn spin magnetic moment is very localized due to the exclusion of the spin-down electrons at the Mn site and amounts to about 3.7 μ_B in the case of NiMnSb. In the case of CoMnSb the increased hybridization between the Co and Mn spin-down electrons decreased the Mn spin moment to about 3.2 μ_B. In the case of the full-Heusler alloys each Mn atom has eight Co atoms as first neighbors instead of four as in CoMnSb and the above hybridization is very important decreasing even further the Mn spin moment to less than 3 μ_B except in the case of Co_2MnSn where it is comparable to the CoMnSb compound. The Co atoms are ferromagnetically coupled to the Mn spin moments and they posses a spin moment that varies from $\sim$0.7 to 1.0 μ_B, while the *sp* atom has a very small negative moment which is one order of magnitude smaller than the Co moment. The negative sign of the induced *sp* moment characterizes most of the studied full and half Heusler alloys with very few exceptions. The compounds containing Al and Ga have 28 valence electrons and the ones containing Si, Ge and Sn 29 valence electrons. The first compounds have a total spin moment of $4\mu_B$ and the second ones of 5 μ_B which agree with the experimental deduced moments of these compounds [57]. So it seems that the total spin moment, M_t, is related to the total number of valence electrons, Z_t, by the simple relation: $M_t = Z_t - 24$, while in the half-Heusler alloys the total magnetic moment is given by the relation $M_t = Z_t - 18$. In the following Section I will analyze the origin of this rule.

4. Origin of the gap and Slater-Pauling behavior

4.1 Origin of the gap: Half-Heusler alloys

In the Heusler alloys the gap basically arises from the covalent hybridization between the lower-energy *d* states of the high-valent transition metal (TM) atom like Ni or Co and the higher-energy *d* states of the lower-valent TM atom like Mn or Cr, leading to the formation of bonding and antibonding bands with a gap in between. The bonding hybrids are located mainly at the high-valent TM atom site and the unoccupied antibonding states at the lower-valent TM atom site, *e.g* in Fig. 4 the minority occupied bonding *d* states are mainly of Ni character while the unoccupied antibonding states are mainly of Mn character. Similarly to the situation of the elemental and compound semiconductors, these structures are particularly stable when only the bonding states are occupied. In binary TM alloys this situation usually does not occur, since the total charge is too large to be accommodated in the bonding hybrids only, or, if this is possible, the covalent hybridization is not sufficient to form a gap.

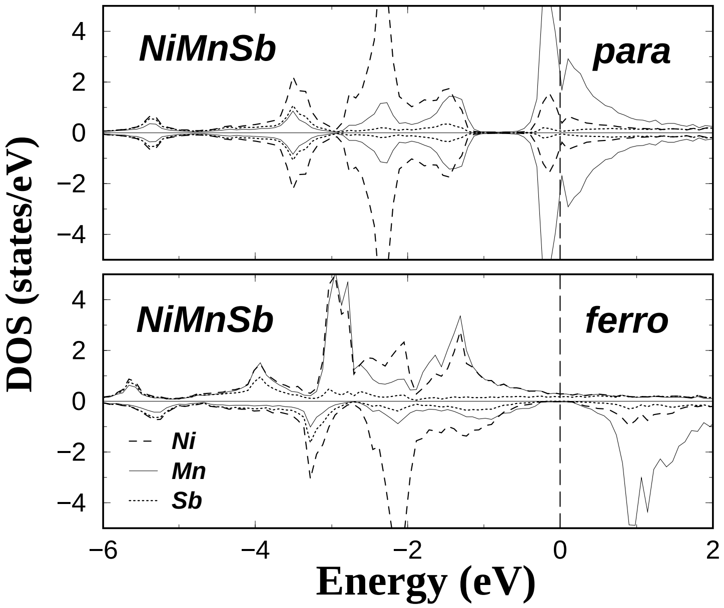

Figure 4. Ferro- and para-magnetic atomic- and spin-resolved density of states of NiMnSb. Note that the bonding d states are mainly of Ni character, while the antibonding d states are mainly of Mn character, and they are separated by a gap.

For these reasons the sp-elements like Sb play an important role for the existence of the Heusler alloys with a gap at the E_F. While an Sb atom has 5 valence electrons ($5s^2$, $5p^3$), in the NiMnSb compound each Sb atom introduces a deep lying s-band, at about -12 eV, and three p-bands below the center of the d-bands. These bands accommodate a total of 8 electrons per unit cell, so that formally Sb acts as a triple charged Sb^{-3} ion. Analogously, a Te-atom behaves in these compounds as a Te^{-2} ion and a Sn-atom as a Sn^{-4} ion. This does not mean, that locally such a large charge transfer exists. In fact, the s- and p-states strongly hybridize with the TM d-states and the charge in these bands is delocalized and locally Sb even looses about one electron. What counts is that the s- and p-bands accommodate 8 electrons per unit cell, thus effectively reducing the d-charge of the TM atoms. Since the bonding d-bands introduced above can accommodate 10 electrons, one expects therefore that the non-magnetic Heusler alloys with 18 valence electrons per unit cell are particularly stable and have a gap at E_F, i.e. are semiconducting, which requires, of course, a sufficient strong covalency between the TM partners for the gap to exist. This “18-electron rule” was recently derived by Jung *et al.* based on ionic arguments [58]. Examples for the semiconducting $C1_b$ Heusler alloys are CoTiSb and NiTiSn [59]. In the case of CoTiSb the Sb atom brings 5 valence electrons and the Co and Ti atoms 9 and 4, respectively. Of the 13 TM electrons 3 are catched by the Sb atom, so that the remaining 10 electrons just fill the bonding d-bands. In the case of NiTiSn, the Ni atom brings in one more electron than Co, but the Sn atom with 4 valence electrons catches away 4 *d*-electrons, so that again 10 electrons remain for the bonding *d* bands.

Also for systems with more (or less) than 18 electrons, the gap can still exist. These systems are no longer semiconducting and loose part of the stability, since then also anti-bonding states are occupied (or not all bonding states are occupied). An example is the paramagnetic DOS of NiMnSb, shown in Fig. 4. Of the 22 valence electrons, four have to be accommodated in the antibonding *d*-bands. The high DOS at E_F signalizes that the Stoner criterium is met so that in the $C1_b$ structure NiMnSb should be a ferromagnet. Of the possible magnetic states, the half-metallic states, as shown by the spin polarized DOS of NiMnSb in Fig. 4, is particularly favored due to the gap at E_F in the minority band. Thus for these half-metallic Heusler alloys the 18-electron rule for the semiconducting Heusler is replaced by a 9-electron rule for the number of minority electrons. By denoting the total number of valence electrons by Z_t, being an integer itself, the total moment M_t per unit cell is then given by the simple rule $M_t = Z_t - 18$ in μ_B, since $Z_t - 18$ gives the number of uncompensated spins. Thus the total moment M_t is an integer quantity, assuming the values 0, 1, 2, 3, 4 and 5 if $Z_t \geq 18$. The value 0 corresponds to the semiconducting phase and the value 5 to the maximal moment when all 10 majority *d*-states are filled. The above relation naturally explains why *e.g.* NiMnSb with $Z_t = 22$ has a total moment of 4 μ_B, CoMnSb with $Z_t = 21$ a moment of 3 μ_B and FeMnSb with $Z_t = 20$ a moment of 2 μ_B.

4.2 Origin of the gap: Full-Heusler alloys

As I mentioned above in section 3.2, the total spin magnetic moments of the Co_2MnZ compounds follow the $M_t = Z_t - 24$ rule. Similarly to the above discussion on the half-Heusler alloys this rule means that there are 12 occupied spin-down states, as the total moment, which is the number of uncompensated spins, is given by the total number of valence electrons Z_t minus two times the number of minority electrons. It is important in order to explain the properties of these compounds to take into account firstly the interactions between the two inequivalent Co sites and then their interaction with the Mn or the *sp* atom (see Fig. 5a), as was also the case for the Fe_2MnZ compounds [38]. Firstly, similar to the half-Heusler alloys the *sp* atom creates one *s* band and three *p* bands which are fully occupied. The *s* electrons transform following the Γ_1 representation; I do not show this band in Fig. 5b as it very low in energy and is well separated by the other bands. The *p* electrons of the *sp* atom transform following the Γ_{15} representation and they hybridize with *p* electrons of the Mn and of the Co that transform with the same representation. As can be seen in the band structure, these bands are lower than the bands that have mainly *d* character but they are not well separated by them (there is a band crossing along the ΓK direction). As in the half-Heusler alloys, the 4 *sp* bands can be only partially filled by the *n* valence electrons of the *sp* atom ($n = 3$ for Al, Ga or 4 for Si Ge and Sn), so that an additional $8 - n$ *d* electrons are accommodated in these bands (4 *d*-electrons in the case of Co_2MnGe or 5 *d*-electrons for Co_2MnAl). Therefore in both kind of Heusler alloys the effective number of *d* electrons (in the higher lying *d* bands) can be controlled by the valence of the *sp* atom. This is a very unusual behavior for metallic systems, which can be used to engineer Heusler alloys with very different magnetic properties (see next section). Before going on discussing the behavior of the *d* orbitals we should note that the band structure seems to be symmetric along the LΓ and

KX directions due to the backfolding of the bands caused by the two Co atoms per unit cell.

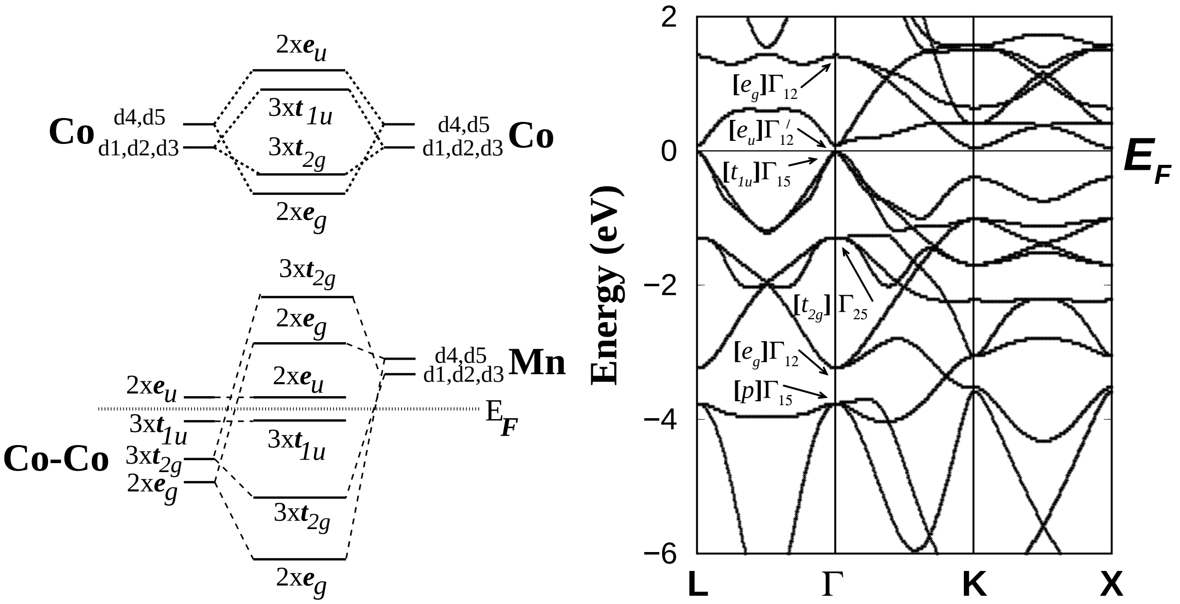

Figure 5. (a)Possible hybridizations between spin-down orbitals sitting at different sites in the case of the Co_2MnGe compound. To explain the properties of the full Heusler alloys, firstly I consider the hybridization between the two different Co atoms and afterwards the hybridization with the Mn atom. The coefficient represents the degeneracy of each orbital. (b) Spin-down band structure of the Co_2MnGe compound. The indirect gap, present in the half-Heusler alloys, is practically destroyed. In brackets I present the type of orbitals transforming following each representation.

In the case of the half-Heusler alloys, like CoMnSb, there is only one Co atom per unit cell and its d valence electrons are hybridizing with the Mn ones creating five bonding states below the Fermi level and five antibonding ones above the Fermi level. In the full-Heusler alloys the existence of the second Co atom makes the physics of these systems more complex. In order to discuss the behavior of the d electrons in the full Heusler alloys I have drawn schematically in Fig. 5a the possible hybridizations between the different atoms. The $d_{1\ldots5}$ orbitals correspond to the d_{xy}, d_{yz}, d_{zx}, $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbitals, respectively. The symbol e_g means that the orbital transform following the E_g representation and in the band structure I also present the representations of the symmetry group of the Γ point that has been introduced in Ref. [60]. Note that due to symmetry, the e_g orbitals at the Co site can only couple with e_g orbitals at the other Co site or at the Mn site. The same applies for the t_{2g} orbitals. Looking at Fig. 5a I see firstly that when two neighboring Co atoms interact, their d_4 and d_5 orbitals form bonding e_g and antibonding e_u states (the coefficient in front of each orbital is the degeneracy of this orbital). The d_1, d_2 and d_3 orbitals of each Co also hybridize creating a triple degenerated bonding t_{2g} orbital and a triple degenerated antibonding t_{1u} orbital. As mentioned above the $L2_1$ structure obeys the tetrahedral symmetry T_d but if only the Co sites are considered, they form a cubic lattice obeying the octahedral symmetry O_h. The e_u and t_{1u} hybrids obey the higher O_h symmetry and for symmetry reasons they cannot couple to either the d states of the Mn nor the d states of the Ge atoms.

As I show in the second part of Fig. 5a, the double degenerated e_g orbitals hybridize with the d_4 and d_5 of the Mn that transform also with the same representation. They create a double degenerated bonding e_g state that is very low in energy and an antibonding one that is unoccupied and above the Fermi level. The $3 \times t_{2g}$ Co orbitals couple to the $d_{1,2,3}$ of the Mn and create 6 new orbitals, 3 of which are bonding and are occupied and the other three are antibonding and high in energy. Finally the $2 \times e_u$ and $3 \times t_{1u}$ Co orbitals cannot couple with any of the Mn d orbitals as there are none transforming with the u representations. With respect to the Mn and the Ge atoms these states are therefore non-bonding. The t_{1u} states are below the Fermi level and they are occupied while the e_u are just above the Fermi level. Thus in total 8 minority d bands are filled and 7 are empty. Our description is somewhat different from the one in Ref. [38] where it has been assumed that the orbitals just below the Fermi level are also t_{2g} and not t_{1u} as in my case. To elucidate this difference I have drawn in Fig. 6 the atomic-resolved d DOS projected on the double degenerated and the triple degenerated representations. Although I cannot distinguish in my projection the t_{2g} from the t_{1u} and the e_g from the e_u, around the Fermi level the Mn atom presents a broad spin-down gap which is not present at the Co sites. So the minority states around the gap are localized at the Co and do not couple to Mn, and the only states that have this property are the t_{1u} and the e_u. Thus the peak below the Fermi level is the $3 \times t_{1u}$ state and the peak just above the Fermi level is the $2 \times e_u$ state. This also explains why the gap is small. The two Cobalt atoms are second neighbors and their hybridization is not so strong and the splitting of the states is small and thus the energy distance between the t_{1u} levels and the e_u ones is small. As these states do not hybridize with the Mn states their splitting does not change and the gap is considerably smaller than the one in the half-Heusler alloys. In the latter compounds I have only one Co atom per unit cell coupling to the Mn atom and so the t_{1u} and the e_u states are absent and only the e_g and t_{2g} survive. Therefore a large gap exists in the half-Heusler alloys and the minority valence bands contain 9 electrons: $1 \times s$, $3 \times p$ and $5 \times d$.

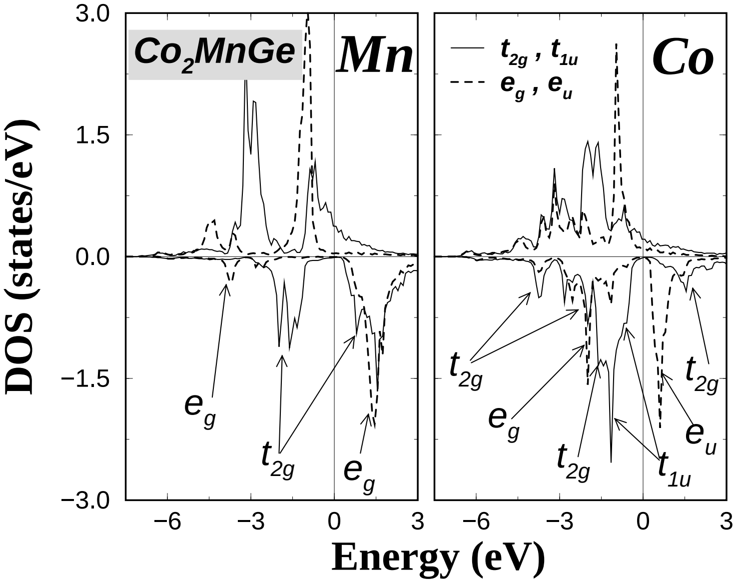

Figure 6. Projected d DOS on the double and on the triple degenerated representations for each atom in the Co$_2$MnGe compound. I also give the character of each peak for the spin-down states. Notice that

in the minority bands around the Fermi level there are only Co states.

To summarize, in the case of the full-Heusler alloys I have 8 occupied minority d states per unit cell: the double degenerated e_g very low in energy, the triple degenerated t_{2g} orbital and finally the triple degenerated t_{1u} just below the Fermi level. Thus in total I have 12 minority occupied states per unit cell, one with s character, three with p character and 8 with d character. Therefore the total moment obeys the simple rule $M_t = Z_t - 24$, as compared to $M_t = Z_t - 18$ for the half-Heusler alloys. Note here that as shown in Fig. 5a I have in total 15 spin-down d states, meaning 30 in total if I take into account both spin directions, so the states count is correct as each of the two Co atoms and the Mn one contributes totally 10 d states. I can trace these states also in the spin-down band structure analyzing the character of each band at the Γ point. Firstly as said above I have a s like band not shown in Fig. 5b with a Γ_1 state at the Γ point and then I find at Γ a triple degenerated point that has the Γ_{15} representation corresponding to the p like orbitals. Above this point there is a double-degenerated Γ_{12} point which corresponds to the e_g orbitals while the other e_g orbitals for Co_2MnGe are found above the Fermi level and also above the unoccupied e_u orbitals that correspond to the double degenerated point with the Γ'_{12} symmetry. Finally, there are two triple degenerated points Γ_{25} and Γ_{15} which correspond to the occupied t_{2g} and t_{1u} orbitals, respectively, while the other unoccupied t_{2g} orbitals (Γ_{25}) are high in energy and are not shown in the figure.

From the above discussion I find that in the minority band 7 d states above E_F are unoccupied. Thus the largest possible moment, which a full-Heusler alloys can have, is 7 μ_B, since in this case all majority d states are filled. This is different from the half-Heusler compounds which have five empty d-states in the minority band and therefore a maximum moment of 5 μ_B.

4.3 Slater-Pauling Behavior

As I discussed in Section 4.1 both the half- and the full-Heusler compounds follow the well-known later-Pauling behavior for the binary transition metal (TM) alloys [52]. In such a picture the total spin moment M_t scales with the total number of valence electrons Z_t. The difference between the different alloys is that in the Heusler alloys the TM minority population is fixed at 5 or 8 for the half and full alloys, respectively, and the screening is achieved by filling the majority band, while in the binary TM alloys the majority band is filled and the charge neutrality is achieved by filling the minority states. As a result, for the Heusler alloys the moment increases with the total charge Z_t, while in the TM binary alloys it decreases with increasing Z_t, since the total moment is given by $M_t = 10 - Z_t$.

In Fig. 7 I have gathered the calculated total spin magnetic moments for the half-Heusler alloys I studied as a function of the total number of valence electrons. With dashed line I represent the rule $M_t = Z_t - 18$ obeyed by these compounds. In such a picture the total moment M_t is an integer quantity, assuming the values 0, 1, 2, 3, 4 and 5 if $Z_t \geq 18$. The value 0 corresponds to the semiconducting phase and the value 5 to the maximal moment when all 10 majority d-states are filled. Firstly I varied the valence of the lower-valent (*i.e.* magnetic) transition metal atom. Thus I substitute V, Cr and Fe for Mn in the NiMnSb and CoMnSb compounds using the experimental lattice constants of the two Mn compounds. For all these compounds I find that the total spin moment scales accurately with the total charge and they all present the half-ferromagnetism.

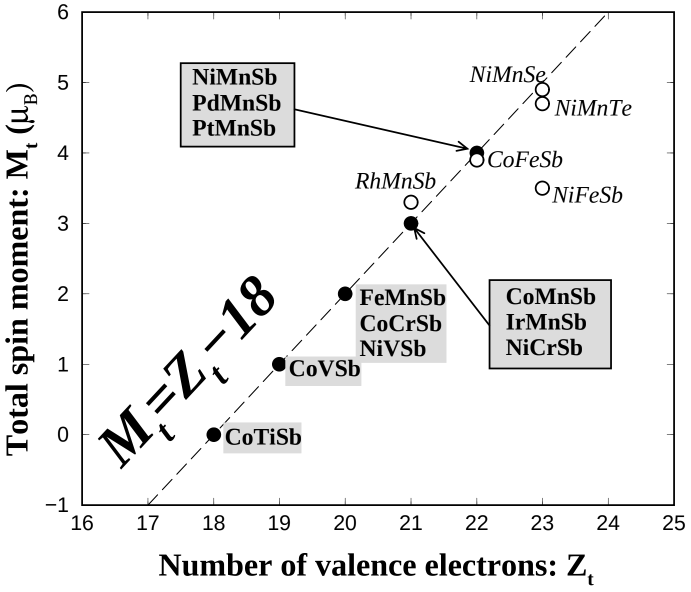

Figure 7. Calculated total spin moments for all the studied half Heusler alloys. The dashed line represents the Slater-Pauling behavior. With open circles we present the compounds deviating from the SP curve.

As a next test I have substituted Fe for Mn in CoMnSb and NiMnSb, but both CoFeSb and NiFeSb loose their half-ferromagnetic character. In the case of NiFeSb the majority d-states are already fully occupied as in NiMnSb, thus the additional electron has to be screened by the minority d-states, so that the Fermi level falls into the minority Fe states and the half-metallicity is lost; for half-metallicity a total moment of 5 μ_B would be required which is clearly not possible. For CoFeSb the situation is more delicate. This system has 22 valence electrons and if it would be a half-ferromagnet it should have a total spin-moment of 4 μ_B like NiMnSb. In reality my calculations indicate that the Fermi level is slightly above the gap and the total spin-moment is slightly smaller than 4 μ_B. The Fe atom possesses a comparable spin-moment in both NiFeSb and CoFeSb compounds contrary to the behavior of the V, Cr and Mn atoms. Except NiFeSb other possible compounds with 23 valence electrons are NiMnTe and NiMnSe. I have calculated their magnetic properties using the lattice constant of NiMnSb. As shown in Fig.7, NiMnSe almost makes the 5 μ_B (its total spin moment is 4.86 μ_B) and it is nearly half-metallic. NiMnSe as was also the case for NiMnAs shows big changes in the majority band compared to NiMnSb or NiMnTe, since antibonding p-d states, which are usually above E_F, are shifted below the Fermi level, thus increasing the total moment to nearly 5 μ_B.

Following the discussion of the previous section I will go on investigating the Slater-Pauling behavior of the full-Heusler alloys and in Fig. 8 I have plotted the total spin magnetic moments for all the compounds under study as a function of the total number of valence electrons. The dashed line represents the rule: $M_t = Z_t - 24$. In the following I will analyze some of these results. Overall I see that many of my results coincide with the Slater-Pauling curve. Some of the Rh compounds show small deviations which are more serious for the Co_2TiAl compound. I see that there is no compound with a total spin moment of 7 μ_B or even 6 μ_B. Moreover I found also examples of half-metallic materials with less than 24 electrons, Mn_2VGe with 23 valence electrons and Mn_2VAl with 22 valence electrons. Firstly, I have calculated the spin moments of the compounds Co_2YAl where Y= Ti, V, Cr, Mn and Fe. The compounds containing V, Cr and Mn show a similar behavior. As I substitute Cr for Mn, that has one valence electron less than Mn, I depopulate one Mn spin-up state and thus the spin moment of Cr is around 1 μ_B smaller than the Mn one while the Co moments are practically the same for both compounds. Substituting V for Cr has a larger effect since also the Co spin-up DOS changes slightly and the Co magnetic moment is increased by about 0.1 μ_B compared to the other two compounds and V possesses a small moment of 0.2 μ_B. This change in the behavior is due to the smaller hybridization between the Co atoms and the V compared to the Cr and Mn atoms. Although all three Co_2VAl, Co_2CrAl and Co_2MnAl compounds are on the SP curve as can be seen in Fig. 8, this is not the case for the compounds containing Fe and Ti. If the substitution of Fe for Mn followed the same logic as the one of Cr for Mn then the Fe moment should be around 3.5 μ_B which is a very large moment for the Fe site. Therefore it is energetically more favorable for the system that also the Co moment is increased, as it was also the case for the other systems with 29 electrons like Co_2MnSi, but while the latter one makes it to 5 μ_B, Co_2FeAl reaches a value of 4.9 μ_B. In the case of Co_2TiAl, is is energetically more favorable to have a weak ferromagnet than an integer moment of 1 μ_B as it is very difficult to magnetize the Ti atom. Even in the case of the Co_2TiSn the calculated total spin magnetic moment of 1.78 μ_B (compared to the experimental value of 1.96 μ_B [61]) arises only from the Co atoms as was also shown experimentally by Pendl *et al.* [62], and the Ti atom is practically paramagnetic and the latter compound fails to follow the SP curve.

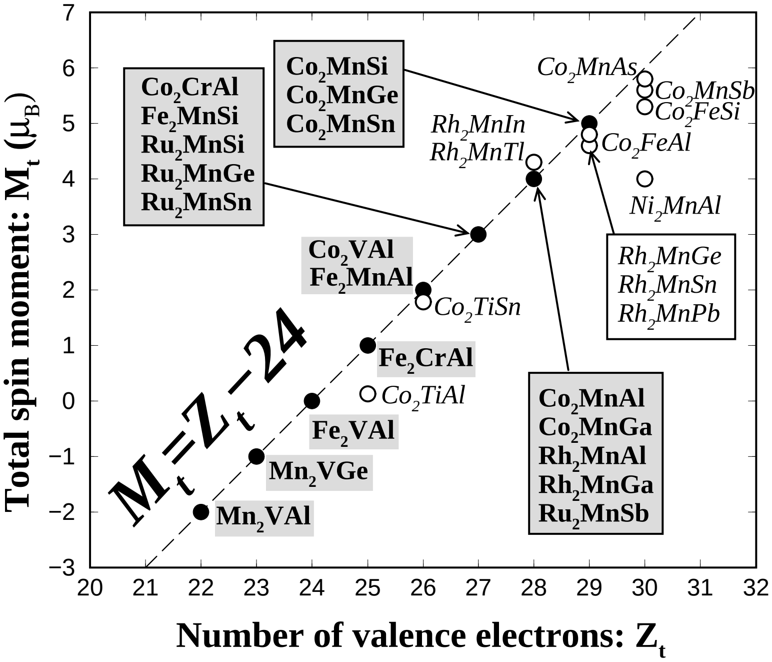

Figure 8. Calculated total spin moments for all the studied full Heusler alloys. The dashed line represents the Slater-Pauling behavior. With open circles we present the compounds deviating from the SP curve.

As a second family of materials I have calculated also the compounds containing Fe. Fe_2VAl has in total 24 valence electrons and is a semimetal, *i.e.* paramagnetic with a very small DOS at the Fermi level, as it is already known experimentally [63]. All the studied Fe compounds follow the SP behavior as can be seen in Fig. 8. In the case of the Fe_2CrAl and Fe_2MnAl compounds the Cr and Mn atoms have spin moments comparable to the Co compounds and similar DOS. In order to follow the SP curve the Fe in Fe_2CrAl is practically paramagnetic while in Fe_2MnAl it has a small negative moment. When I substitute Si for Al in Fe_2MnAl, the extra electron exclusively populates Fe spin-up states and the spin moment of each Fe atom is increased by 0.5 μ_B contrary to the corresponding Co compounds where also the Mn spin moment was considerably increased. Finally I calculated as a test Mn_2VAl and Mn_2VGe that have 22 and 23 valence electrons, respectively, to see if I can reproduce the SP behavior not only for compounds with more than 24, but also for compounds with less than 24 electrons. As I have already shown Fe_2VAl is paramagnetic and Co_2VAl, which has two electrons more, has a spin moment of 2 μ_B. Mn_2VAl has two valence electrons less than Fe_2VAl and its total spin moment is -2 μ_B and thus it follows the SP behavior. To my knowledge there is no compound with 23 valence electrons, which has been studied experimentally, so I decided to calculate Mn_2VGe using the lattice constant of Mn_2VAl. I found that adding one electron to Mn_2VAl results in a decrease of the absolute value of both the Mn and V spin moments (note that V and Mn are antiferromagnetically coupled) so that the resulting Mn_2VGe total spin magnetic moment is -1 μ_B following the SP curve as can be also seen in Fig. 8.

To investigate further the Slater-Pauling behavior of the full-Heusler alloys I studied the ones containing a $4d$ transition metal atom. The Ru compounds are antiferromagnets with Néel temperatures that reach room temperature [64]. I have calculated their properties assuming that they are ferromagnets. Contrary to the Ru compound which follow the SP curve, in the case of the Rh ones [34, 65] only Rh_2MnAl and Rh_2MnGa are exactly on the SP curve. The rest of them present small deviations.

As I have already mentioned the maximal moment of a full-Heusler alloy is seven μ_B, and should occur, when all 15 majority d states are occupied. Analogously for a half-Heusler alloy the maximal moment is 5 μ_B. However this limit is difficult to achieve, since due to the hybridization of the d states with empty *sp*-states of the transition metal atoms (sites X and Y in Fig. 1), d-intensity is transferred into states high above E_F, which are very difficult to occupy. Although in the case of half-Heusler alloys, I could identify systems with a moment of nearly 5 μ_B, the hybridization is much stronger in the full-Heusler alloys so that a total moment of 7 μ_B seems to be impossible. Therefore I restrict my search to possible systems with 6 μ_B, *i.e.* systems with 30 valence electrons, but as shown also in Fig. 8, none of them makes exactly the 6 μ_B. Co_2MnAs shows the largest spin moment: 5.8 μ_B. If I increase its lattice constant by 3% the Fermi level moves deeper in energy and now it falls within the gap and the total spin moment reaches the ideal value of 6 μ_B. So if Co_2MnAs can be grown on top of a substrate with the appropriate lattice constant using a technique like Molecular Beam Epitaxy, it is possible to get a material with a total spin moment of 6 μ_B. From the trends of Co_2MnSb and Co_2MnAs, I expect that Co_2MnP, if it exists, should have a total moment of 6 μ_B.

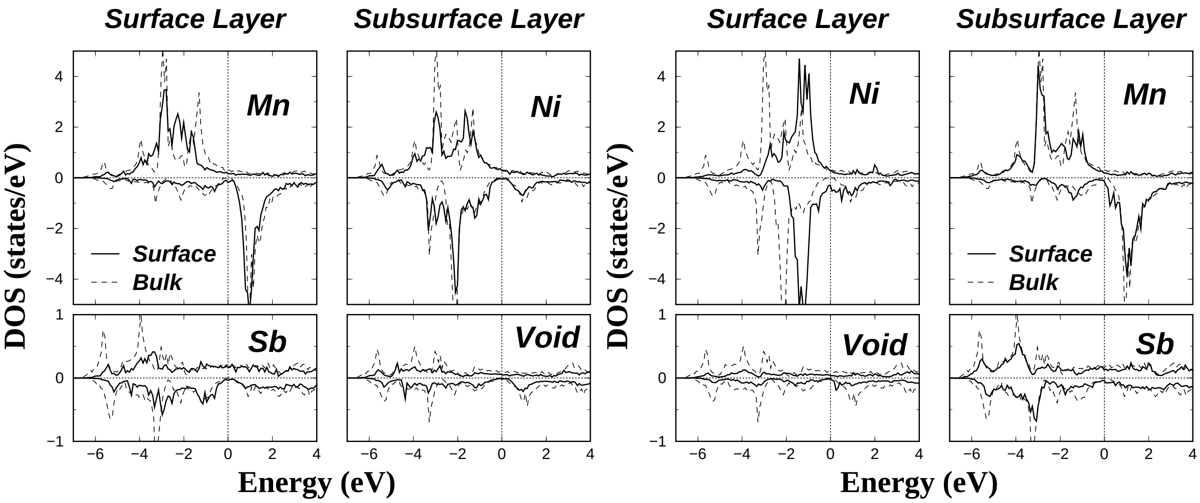

Figure 9. Spin- and atom-projected DOS for the MnSb-terminated NiMnSb(001) surface (left panel) and for the Ni-Void terminated (001) surface (right panel). The dashed lines give the local DOS of the atoms in the bulk.

5. Properties of the (001) Surfaces

5.1 Half-Heusler Alloys

In the first part of this section I concentrate on the half-Heusler compounds. I used the NiMnSb compound as the model system. As shown by Jenkins and King [31], the MnSb terminated surface of NiMnSb shows very small relaxations, while no information is available for the Ni-terminated surface which in principle should show large relaxations due to the vacant site at the surface. In my study I assume an "ideal" epitaxy in both cases. In the left panel of Fig. 9, I present the atom- and spin-projected density of states (DOS) for the Mn and Sb atoms in the surface layer and the Ni and vacant site in the subsurface layer for the MnSb terminated NiMnSb(001) surface, and in the right panel of the same figure I present the atom- and spin-projected DOS of the surface and the subsurface layers for the Ni terminated surface. In both cases I compare the surface DOS with the bulk calculations (dashed line).

In the case of the MnSb terminated surface the DOS with the exception of the gap area is very similar to the bulk calculations. The Ni atom in the subsurface layer presents practically a half-ferromagnetic character with an almost zero spin-down DOS, while for the bulk there is an absolute gap. The spin-down band of the vacant site also presents a very small DOS around the Fermi level. The Mn and Sb atoms in the surface layer show more pronounced differences with respect to the bulk, and within the gap there is a very small Mn-d and Sb-p DOS. These states are strongly localized at the surface layer as at the subsurface layer there is practically no states inside the gap. This is in agreement with previous pseudopotentials calculations that showed that the surface states at the case of the MnSb-terminated NiMnSb(001) surface are localized at the surface layer [31]. Our results are in agreement with the experiments of Ristoiu *et al.* [24] who in the case of a MnSb well ordered (001) surface measured a high spin-polarization.

It is also interesting to examine the spin-polarization at the Fermi level. In Table 2 we have gathered the number of spin-up and spin-down states at the Fermi level for each atom at the surface and the subsurface layer for both terminations. I calculated the spin-polarization as the ratio between the number of spin-up states minus the number of spin-down states over the total DOS at the Fermi level. P_1 corresponds to the spin-polarization when I take into account only the surface layer and P_2 when I also include the subsurface layer. P_2 represents quite well the experimental situation as the spin-polarization in the case of films is usually measured by inverse photoemission which probes only the surface of the sample [66]. In all cases the inclusion of the subsurface layer increased the spin-polarization. In the case of the Ni terminated surface, the spin-up DOS at the Fermi level is equal to the spin-down DOS and the net polarization P_2 is zero. In the case of the MnSb terminated surface the spin-polarization increases and now P_2 reaches a value of 38%, which means that the spin-up DOS at the Fermi level is about two times the spin-down DOS. As can be seen in Table 2 the main difference between the two different terminations is the contribution of the Ni spin-down states. In the case of the MnSb surface the Ni in the subsurface layer has a spin-down DOS at the Fermi level of 0.05 states/eV, while in the case of the Ni-terminated surface the Ni spin-down DOS at the Fermi level is 0.40 states/eV decreasing considerably the spin-polarization for the Ni terminated surface; the Ni spin-up DOS is the same for both terminations. It is interesting also to note that for both surfaces the net Mn spin-polarization is close to zero while Sb atoms in both cases show a large spin-polarization and the number of the Sb spin-up states is similar to the number of Mn spin-up states, thus Sb and not Mn is responsible for the large spin-polarization of the MnSb layer in both surface terminations. The calculated P_2 value of 38% for the MnSb terminated surface is smaller than the experimental value of 67% obtained by Ristoiu and collaborators [24] for a thin-film terminated in a MnSb stoichiometric alloy surface layer. But experimentally no exact details of the structure of the film are known and the comparison between experiment and theory is not straightforward.

The other half-Heusler alloys present surface properties similar to the ones of NiMnSb. In the case of the Co terminated CoMnSb surface as it was the case for the Ni terminated surface there is a shift of the Co spin-down DOS towards higher energies and the Co spin-down DOS at the Fermi level is very high and thus P_2 is negative, meaning that the spin-down DOS is larger than the spin-up DOS at the Fermi level. In the case of the MnSb terminated CoMnSb surface, the Co atom in the subsurface layer has practically zero spin-down DOS and P_2 reaches 46%. In the case of PtMnSb, Pt does not show such a pronounced difference between the two surface terminations as the Co atom because it has practically all its *d* states filled and the DOS near the Fermi level is small. But also for PtMnSb the MnSb terminated surface shows a very large spin-polarization comparable to the one of CoMnSb, while the Pt terminated (001) surface shows a positive spin-polarization contrary to the vanishing net spin-polarization of the Ni surface and the negative one of the Co terminated surface.

Table 2. Atomic-resolved spin-up and spin-down DOS at the Fermi level in states/eV units. They are presented as ratios spin-up over spin-down. Polarization ratios at the Fermi level are calculated taking into account only the surface layer P_1, and both the surface and subsurface layers P_2.

	MnSb-termination					
	Surface Layer		Subsurface Layer			
	Mn (↑ / ↓)	Sb (↑ / ↓)	Ni[Co,Pt] (↑ / ↓)	Void (↑ / ↓)	P_1 ($\frac{\uparrow-\downarrow}{\uparrow+\downarrow}$)	P_2 ($\frac{\uparrow-\downarrow}{\uparrow+\downarrow}$)
NiMnSb	0.16/0.19	0.17/0.03	0.28/0.05	0.05/0.02	26%	38%
CoMnSb	0.23/0.27	0.16/0.07	0.91/0.15	0.07/0.02	6%	46%
PtMnSb	0.21/0.24	0.31/0.06	0.38/0.04	0.08/0.02	26%	46%
	Ni(Co,Pt)Void-termination					
	Subsurface Layer		Surface Layer			
	Mn (↑ / ↓)	Sb (↑ / ↓)	Ni[Co,Pt] (↑ / ↓)	Void (↑ / ↓)	P_1 ($\frac{\uparrow-\downarrow}{\uparrow+\downarrow}$)	P_2 ($\frac{\uparrow-\downarrow}{\uparrow+\downarrow}$)
NiMnSb	0.18/0.16	0.13/0.05	0.27/0.40	0.04/0.02	−16%	0%
CoMnSb	0.55/0.68	0.12/0.07	0.54/1.15	0.05/0.04	−34%	−22%
PtMnSb	0.18/0.14	0.21/0.07	0.30/0.24	0.05/0.02	14%	22%

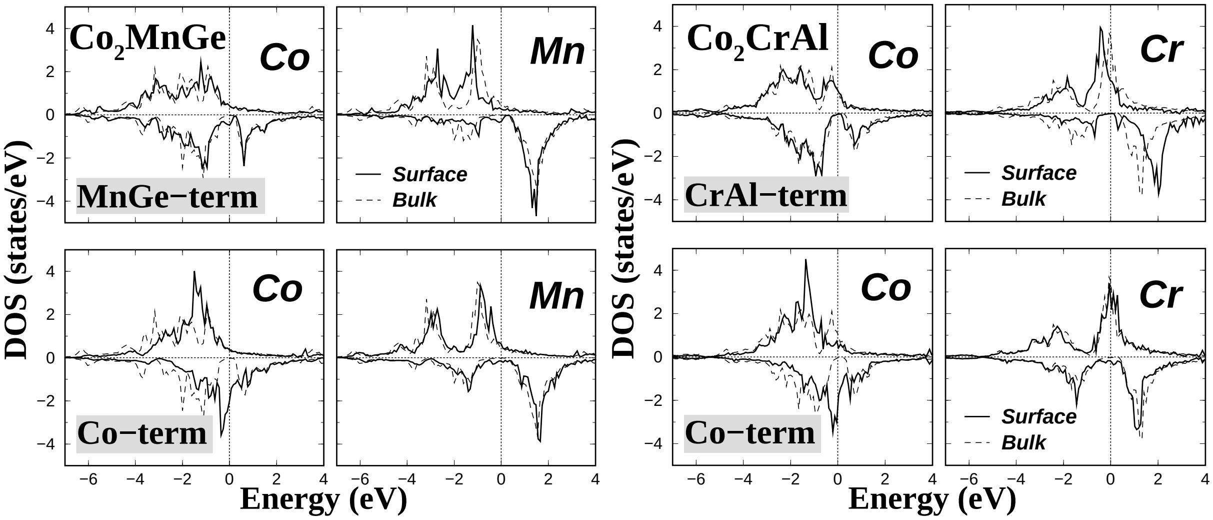

Figure 10. Atom- and spin-projected DOS for the Mn atom in the surface and the Co atom in the subsurface layer in the case of the MnGe terminated Co_2MnGe (001) surface (left upper panel) and the Co atom in the surface layer and the Mn atom in the subsurface for the Co terminated surface (left bottom panel). In the right panel similar DOS for the Co_2CrAl compound. With dashed line the bulk results.

5.2 Full-Heusler Alloys

I continue my study with the full-Heusler alloys and concentrate mainly on the Co_2MnGe, Co_2MnSi and Co_2CrAl alloys. Co_2MnGe and Co_2MnSi present similar surface properties and thus I will discuss in detail only the properties of Co_2MnGe. As shown in Fig. 10, in the case of the Co terminated surfaces all compounds show the same behavior which is similar to the behavior of the Co surface atom in the case of the Co-terminated CoMnSb surface. The lower coordination number of the Co atoms in the surface layer results in smaller covalent hybridization between the Co spin-down d states and the Mn ones and thus there is a practically rigid shift of the spin-down Co d bands towards higher energies, and now the Fermi level falls at the edge of the large peak of the minority spin DOS.

In the case of the MnGe terminated Co_2MnGe (001) surface the behavior is similar to the MnSb terminated surface in the CoMnSb compound. Due to the reduced symmetry (Mn loses two out of the four Co nearest neighbors) the hybridization between the Mn minority d states and the Co ones is reduced, leading to an increase of the Mn spin-moment by about 0.6 μ_B, while the Co atom at the subsurface layer behaves similar to the bulk case. Where the Mn gap was located in the bulk, there is now a small peak due to a d like Mn atomic state that is shifted in energy due to the lower symmetry and which is pinned at the Fermi level. This state although located at the surface layer is not well localized and the Co atoms in the subsurface layer present a similar peak at the Fermi level. Ishida *et al.* [41] have studied the MnSi and MnGe terminated Co_2MnSi and Co_2MnGe surfaces using a 13 layers thick film. They claim that in the case of the MnSi surface the half-ferromagnetic character, which they have calculated for the bulk Co_2MnSi [36], is preserved, while in the case of the MnGe surface, surface states destroy the gap (in the paper they present the results for the MnSi surface and only shortly refer to the MnGe surface). These results are peculiar since they get a similar electronic structure for the bulk compounds and there is no obvious reason obliging only the MnGe surface to present surface states. Mn atoms have the same environment in both cases and the hybridization between Mn and the *sp* atoms is similar for both Ge and Si. A plausible reason for this behavior is the use of the atomic-sphere approximation in their calculations, where the potential and the charge density are supposed to be spherically symmetric. Although this approximation can accurately describe the bulk compounds due to the close-packed structure they adopt, it is not suitable for surfaces where the non-spherical contributions to the potential and the charge density are important.

The case of Co_2CrAl is different from Co_2MnGe. In line with the reduction of the total valence electrons by 2, the Cr moment is rather small (1.54 μ_B) yielding a total moment of only 3 μ_B instead of 5 μ_B for Co_2MnGe. The Co terminated Co_2CrAl(001) surface shows a similar behavior as the corresponding surface of Co_2MnGe, being in both cases dominated by a strong Co peak in the gap region of the minority band. However the CrAl terminated Co_2CrAl surface behaves very differently, being driven by the large surface enhancement of the Cr moment from 1.54 μ_B to 3.12 μ_B. As a consequence the splitting of the Cr peaks in the majority and minority bands is even enlarged and in particular in the minority band the pseudogap is preserved. Thus this surface is a rare case, since for all the other surfaces studied in this paper, the half-metallicity is destroyed by surface states.

In the last part of this section I will discuss the spin-polarization for the surfaces of the full-Heusler alloys. We concentrate on the MnGe and CrAl terminated surfaces as the Co-terminated ones might show large relaxation and thus are not interesting for applications. In Fig. 11, I present the DOS for the atoms in the surface and subsurface layers for both surfaces. In the case of the MnGe terminated surface the surface states completely kill the spin polarization as the majority spin DOS is pretty small. In the case of the CrAl terminated surface the situation is completely different. The minority DOS around the Fermi level is the same for both the bulk and the CrAl surface. Only Al atoms posses surface states. The Fermi level falls within a region of very high Cr and Co majority spin DOS reducing the effect of these surface states and thus 92% of the electrons at the Fermi level are of spin-up character and the surface keeps a high degree of spin-polarization; P_2 reaches 84%.

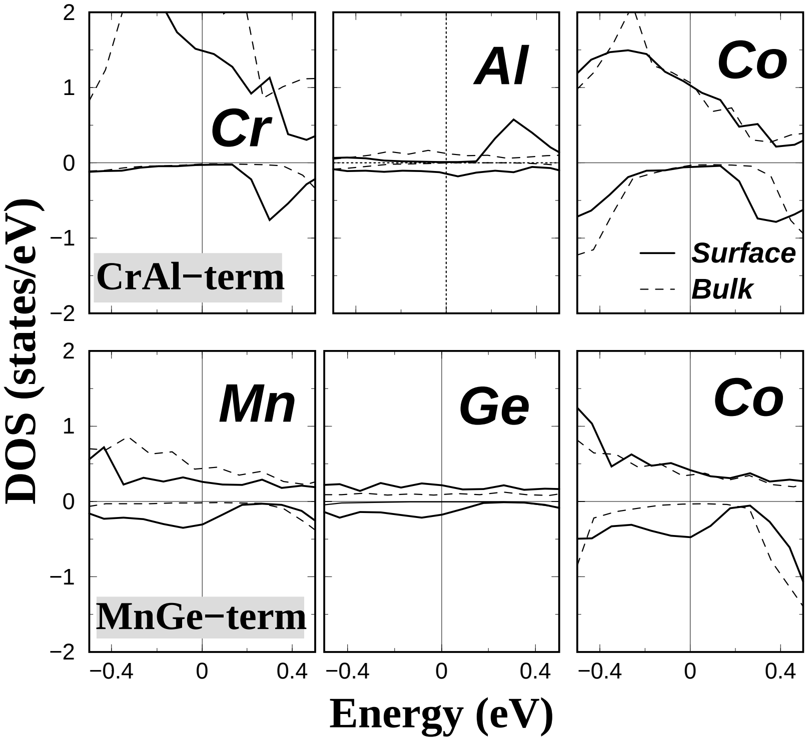

Figure 11. Atom- and spin-projected DOS for the MnGe and CrAl terminated (001) surfaces of Co_2MnGe and Co_2CrAl, respectively. With dashed line: the bulk results.

6. CrAs in the zinc-blende structure

Akinaga and collaborators have managed to grow thin films of CrAs on GaAs(100) substrates by molecular-beam epitaxy [10]. They have found that CrAs is ferromagnetic at room temperature with a T_c larger than 400 K and they have deduced a total spin-magnetic moment of 3 μ_B. Bulk CrAs adopts either the MnP-type structure showing a helimagnetic-paramagnetic transition at 256 K, or it crystallizes as Cr_2As which is an antiferromagnet with a Néel temperature of 393 K. So the structure of the thin film cannot be one of the two stable bulk structures. Akinaga *et al.* have made the assumption that CrAs adopts the zinc-blende (zb) structure of GaAs and using the full-potential linearized augmented-plane-wave (FLAPW) method they have shown that in the ferromagnetic case zb-CrAs would be a half-metal with a total spin magnetic moment of 3 μ_B in agreement with the experiment. Afterwards, Shirai [67] continued the theoretical study of the 3d-transitional monoarsenides and showed that the half-ferromagnetic phase for zb-CrAs should be more stable than the antiferromagnetic solution. He also calculated the theoretical equilibrium lattice constant and found a value of 0.58nm, which lies inbetween the experimental lattice constants of GaAs (0.565nm), AlAs (0.566nm) and InAs (0.606nm).

Using the FSKKR I verified that bulk CrAs is a half-ferromagnet with a total spin moment of 3 μ_B for both the GaAs and InAs lattice constants. The explanation of why there are exactly 3 uncompensated spin states is similar to the one for the half-ferromagnetic Heusler alloys. The As atom in the minority band offers one s band and three p bands low in energy and can accommodate 4 electrons. There are practically no occupied minority d states. The total number of uncompensated spins should be just the total number of valence electrons, 11, minus two times the number of occupied minority states, 2×4=8, and the total spin moment in μ_B would be also (11−8) μ_B= 3 μ_B.

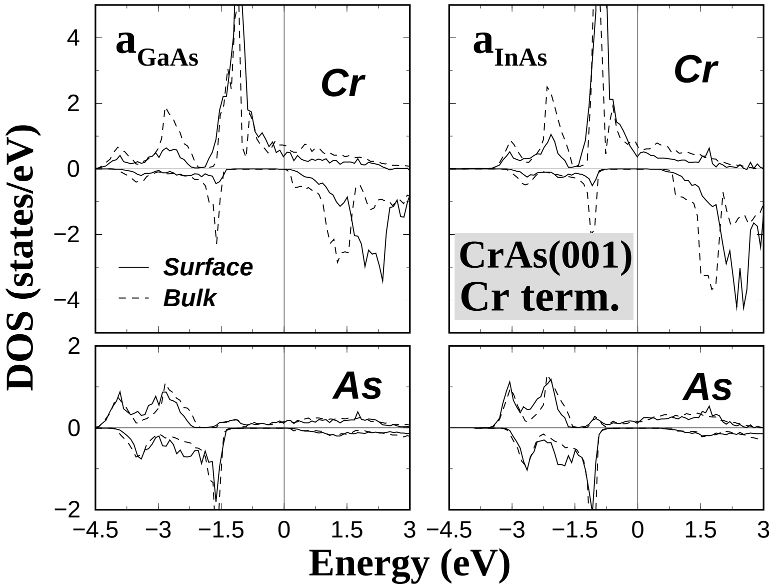

Figure 12. Spin- and atom-resolved DOS of the Cr-terminated (001) surface for the Cr atom at the surface layer and the As atom at the subsurface layer for both the GaAs and InAs lattice constants. The surface DOS are compared to the bulk calculations (dashed lines).

I have also studied the (001) surfaces of CrAs taking into account both the Cr- and As-terminations. I present in Fig. 12 the atomic projected DOS for the Cr atom at the surface and the As atom at the subsurface layer for the Cr-terminated surface and for both the GaAs and InAs lattice constants. There are no surface states within the gap, so this surface is half-ferromagnetic. To our knowledge this is the first case that electronic structure calculations predict a surface of an intermetallic compound to present 100% spin-polarization at the Fermi level. The As-atom at the subsurface layer has the same tetrahedral environment as in the bulk and the amount of electronic charge, which it looses, is similar to the bulk case. However the DOS of the Cr surface is very different, since the unoccupied Cr minority is shifted to higher energies and the Cr admixture in the occupied part of the minority band is decreased. Thus, while the hybridization with the missing As neighbors should decrease the Cr minority peak, this is overcompensated by the increase of the Cr moment by 0.95 μ_B, which shift the Cr peak to higher energies and stabilizes the gap. The same effect is responsible for the high spin-polarization of the CrAl-terminated $Co_2CrAl(001)$ surface (Fig. 10). The conservation of the half-metallic character at the Cr-terminated CrAs(001) surface means that the total moment increases due to the creation of the surface by exactly 1 μ_B.

In the case of the As-terminated (001) surface the situation is not as ideal as in the case of the Cr terminated surface. Now the As dangling bonds create a surface band within the gap that destroys the half-ferromagnetic character. In the case of the InAs lattice constant the gap is only partially destroyed but the Fermi level is below the remaining fully spin-polarized region. Contrary to the Cr-termination the DOS of both the As surface atom and the Cr subsurface atom present large deviations from the bulk case. The As atom at the surface looses ~ 0.4 more electrons than in the bulk CrAs. Its spin magnetic moment is practically doubled. Although the Cr atoms at the subsurface layer present a charge transfer comparable to the bulk calculations, the changes in their DOS are pronounced, the spin imbalance decreases and their magnetic moment is 0.3-0.4 μ_B lower than in the bulk CrAs.

7. Summary

Using the full-potential screened KKR method I studied the bulk and surface properties of both the half and full Heusler alloys identifying a total of 30 half-ferromagnetic compounds. I have shown that in the case of the half-Heusler alloys with 18 valence electrons, like CoTiSb, the *d* states of Co and Ti hybridize forming ten bonding and ten antibonding states. The large covalent hybridization results in a gap between the occupied and the unoccupied states and the Fermi level falls within this gap. The Sb atom creates two *s* and six *p* bands low in energy which accommodate *d* transition metal electrons (Sb atom acts like an anion: Sb^{-3}) reducing the effective valence *d* charge, which can now be accommodated only in the bonding *d* states and CoTiSb is a semiconductor. This behavior of Sb is general for all the *sp* atoms and it is found even when Sb is replaced by Al; in this case the *sp* bands accommodate 5 transition metal *d* electrons and Al acts like an Al^{-5} ion. In the case of compounds with more than 18 electrons like NiMnSb the extra electrons are taken care only by the spin-up states and the minority bands stay unchanged. Thus there are nine occupied spin-down states and the total spin moment per unit cell (M_t) scales with the total number of valence electrons following the relation: $M_t = Z_t - 18$. This is similar to the well-known Slater-Pauling behavior observed for the transition metal binary alloys, except that in this case the total moment decreases with the total number of valence electrons. Thus the total spin moment of NiMnSb which has 22 valence electrons is calculated to be 4 μ_B, the one of CoMnSb (21 valence electrons) 3 μ_B and the spin moment of FeMnSb (20 valence electrons) 2 μ_B. The maximum moment of the half-Heusler alloys is 5 μ_B, since there are five unoccupied minority *d*-states, but this value is difficult to be achieved.

In the case of the full-Heusler alloys like $\mathrm{Co_2MnGe}$, there are in addition to the Co-Mn bonding and antibonding *d*-hybrids, also Co states which cannot hybridize with neither the Mn nor the Ge atoms and are exclusively localized at the Co sites. Thus in addition to the 5 Co-Mn bonding and 5 Co-Mn antibonding states, there exist 5 such "non-bonding" states which are only splitted-up by the weaker Co-Co hybridization into 3 occupied *d* states of t_{1u} symmetry and 2 unoccupied e_u states, which are located just below and just above the Fermi level such that the indirect gap in these materials is tiny. These extra three electrons make that for the full-Heusler alloys there are 12 occupied minority states instead of 9 in the case of the half-Heusler compounds and the relation for the total spin magnetic moment becomes $M_t = Z_t - 24$. Thus systems like Fe_2VAl with 24 valence electrons are semiconductors with a tiny gap, Co_2VAl (26 valence electrons) has a total spin moment of 2 μ_B, Co_2CrAl 3 μ_B, Co_2MnAl 4 μ_B and finally Co_2MnSi which has 29 valence electrons has a total spin moment of 5 μ_B. This law is also valid for compounds with less than 24 electrons, *e.g* Mn_2VGe and Mn_2VAl which have 23 and 22 valence electrons, respectively, have total moments of -1 and -2 μ_B. The maximal total spin moment for these alloys is 7 μ_B, but as has been shown even the 6 μ_B are unlikely to be achieved.

The surfaces of the Heusler alloys in general loose the half-ferromagnetic character of the bulk compounds. The lower coordination of the atoms at the surface leads to a decrease of the hybridization in the minority band resulting in surface states within the gap, which practically kill the high spin-polarization. However the effect of surfaces states can be reduced by the increase of the local moment of the atoms at the surface. Such an example is the CrAl-terminated $Co_2CrAl(001)$ surface where the Cr moment increases from the bulk value of 1.5 μ_B to more than 3 μ_B and the very large spin-up density of states of the Cr atoms at the surface leads to a spin-polarization of 84%. In the case of the Cr-terminated CrAs(001) the surface even retains the half-metallic character of the bulk CrAs in the metastable zinc-blende structure. Thus the large surface enhancement of the Cr atoms stabilizes the gap at the surface.

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References

[1] F. Heusler, Verh. Dtsch. Phys. Ges. **5**, 219 (1903).

[2] P.J. Webster and K.R.A. Ziebeck, in *Alloys and Compounds of d-Elements with Main Group Elements. Part 2.*, edited by H.R.J. Wijn, Landolt-Boörnstein, New Series, Group III, Vol. 19/c (Springer, Berlin), 1988, pp. 75-184.

[3] K.R.A. Ziebeck and K.-U. Neumann, in *Magnetic Properties of Metals*, edited by H.R.J. Wijn, Landolt-Boörnstein, New Series, Group III, Vol. 32/c (Springer, Berlin), 2001, pp. 64-414.

[4] J. Pierre, R.V. Skolozdra, J. Tobola, S. Kaprzyk, C. Hordequin, M.A. Kouacou, I. Karla, R. Currat, and E. Lelièvre-Berna, J. Alloys Comp. **262-263**, 101 (1997).

[5] J. Tobola and J. Pierre, J. Alloys Comp. **296**, 243 (2000).

[6] R.A. de Groot. F.M. Mueller, P.G. van Engen, and K.H.J. Buschow, Phys. Rev. Lett. **50**, 2024 (1983).

[7] S.A. Wolf, D.D. Awschalom, R.A. Buhrman, J.M. Daughton, S. von Molnár, M.L. Roukes, A.Y. Chtchelkanova, and D.M. Treger, Science **294**, 1488 (2001); G.A. Prinz, Science **282**, 1660 (1998); G.A. Prinz, J. Magn. Magn. Mater. **200**, 57 (1999).

[8] R.J. Soulen Jr., J.M. Byers, M.S. Osofsky, B. Nadgorny, T. Ambrose, S.F. Cheng, P.R. Broussard, C.T. Tanaka, J. Nowak, J.S. Moodera, A. Barry, and J.M.D. Coey, Science **282**, 85 (1998).

[9] H. Akai, Phys. Rev. Lett. **81**, 3002 (1998).

[10] H. Akinaga, T. Manago, and M. Shirai, Jpn. J. Appl. Phys. **39**, L1118 (2000).

[11] J.-H. Park, E. Vescovo, H.-J. Kim, C. Kwon, R. Ramesh, and T. Venkatesan, Nature **392**, 794 (1998).

[12] S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990).

[13] K.A. Kilian and R.H. Victora, J. Appl. Phys. **87**, 7064 (2000).

[14] C.T. Tanaka, J. Nowak, and J.S. Moodera, J. Appl. Phys. **86**, 6239 (1999).

[15] J.A. Caballero, Y.D. Park, J.R. Childress, J. Bass, W.-C. Chiang, A.C. Reilly, W.P. Pratt Jr., and F. Petroff, J. Vac. Sci. Technol. A **16**, 1801 (1998); C. Hordequin, J.P. Nozières, and J. Pierre. J. Magn. Magn. Mater. **183**, 225 (1998).

[16] M.M. Kirillova, A.A. Makhnev, E.I. Shreder, V.P. Dyakina, and N.B. Gorina, Phys. Stat. Sol. (b) **187**, 231 (1995).

[17] K.E.H.M. Hanssen and P.E. Mijnarends, Phys. Rev. B **34**, 5009 (1986); K.E.H.M. Hanssen, P.E. Mijnarends, L.P.L.M. Rabou, and K.H.J. Buschow, Phys. Rev. B **42**, 1533 (1990).

[18] W. van Roy, J. de Boeck, B. Brijs, and G. Borghs, Appl. Phys. Lett. **77**, 4190 (2000); J.-P. Schlomka, M. Tolan, and W. Press, Appl. Phys. Lett. **76**, 2005 (2000).

[19] F.B. Mancoff, B.M. Clemens, E.J. Singley, and D.N. Basov, Phys. Rev. B **60**, R12 565 (1999).

[20] W. Zhu, B. Sinkovic, E. Vescovo, C. Tanaka, and J.S. Moodera, Phys. Rev. B **64**, R060403 (2001).

[21] G.L. Bona, F. Meier, M. Taborelli, E. Bucher, and P.H. Schmidt, Sol. St. Commun. **56**, 391 (1985).

[22] J.A. Caballero, A.C. Reilly, Y. Hao, J. Bass, W.P. Pratt, F. Petroff, and J.R. Childress, J. Magn. Magn. Mat. **198-199**, 55 (1999); R. Kabani, M. Terada, A. Roshko, and J.S. Moodera, J. Appl. Phys. **67**, 4898 (1990).

[23] C.T. Tanaka, J. Nowak, and J.S. Moodera, J. Appl. Phys. **81**, 5515 (1997).

[24] D. Ristoiu, J.P. Nozières, C.N. Borca, T. Komesu, H.-K. Jeong, and P.A. Dowben, Europhys. Lett. **49**, 624 (2000); D. Ristoiu, J.P. Nozières, C.N. Borca, B. Borca, and P.A. Dowben, Appl. Phys. Lett. **76**, 2349 (2000); T. Komesu, C.N. Borca, H.-K. Jeong, P.A. Dowben, D. Ristoiu, J.P. Nozières, Sh. Stadler, and Y.U. Idzerda, Phys. Lett. A **273**, 245 (2000).

[25] C.N. Borca, T. Komesu, H.-K. Jeong, P.A. Dowben, D. Ristoiu, Ch. Hordequin, J.P. Nozières, J. Pierre, Sh. Stadler, and Y.U. Idzerda, Phys. Rev. B **64**, 052409 (2001).

[26] I. Galanakis, S. Ostanin, M. Alouani, H. Dreyssé, and J.M. Wills, Phys. Rev. B **61**, 4093 (2000).

[27] E. Kulatov and I.I. Mazin, J. Phys.: Condens. Matter **2**, 343 (1990); S.V. Halilov and E.T. Kulatov, J. Phys.: Condens. Matter **3**, 6363 (1991); X. Wang, V.P. Antropov, and B.N. Harmon, IEEE Trans. Magn. **30**, 4458 (1994). S.J. Youn and B.I. Min, Phys. Rev. B **51**, 10 436 (1995); V.N. Antonov, P.M. Oppeneer, A.N. Yaresko, A.Ya. Perlov, and T. Kraft, Phys. Rev. B **56**, 13 012 (1997).

[28] P. Larson, S.D. Mahanti, and M.G. Kanatzidis, Phys. Rev. B **62**, 12 574 (2000).

[29] D. Orgassa, H. Fujiwara, T.C. Schulthess, and W.H. Butler, Phys. Rev. B **60**, 13 237 (1999).

[30] G.A. Wijs and R.A. de Groot, Phys. Rev. B **64**, *R*020402 (2001).

[31] S.J. Jenkins and D.A. King, Surf. Sci. **494**, L793 (2001).

[32] S.J. Jenkins and D.A. King, Surf. Sci. **501**, L185 (2002).

[33] P.J. Webster, J. Phys. Chem. Solids **32**, 1221 (1971); K. R.A. Ziebeck and P.J. Webster, J. Phys. Chem. Solids **35**, 1 (1974).

[34] J.C. Suits, Phys. Rev. B **14**, 4131 (1976).

[35] J. Kübler, A.R. Williams, and C.B. Sommers, Phys. Rev. B **28**, 1745 (1983).

[36] S. Ishida, S. Akazawa, Y. Kubo, and J. Ishida, J. Phys. F: Met. Phys. **12**, 1111 (1982); S. Ishida, S. Fujii, S. Kashiwagi, and S. Asano, J. Phys. Soc. Jpn. **64**, 2152 (1995).

[37] S. Fujii, S. Sugimura, S. Ishida, and S. Asano, J. Phys.: Condens. Matter **2**, 8583 (1990).

[38] S. Fujii, S. Ishida, and S. Asano, J. Phys. Soc. Jpn. **64**, 185 (1995).

[39] P.J. Brown, K.U. Neumann, P.J. Webster, and K.R.A. Ziebeck, J. Phys.: Condens. Matter **12**, 1827 (2000).

[40] T. Ambrose, J.J. Krebs, and G.A. Prinz, Appl. Phys. Lett. **76**, 3280 (2000); T. Ambrose, J.J. Krebs, and G.A. Prinz, J. Appl. Phys. **87**, 5463 (2000).

[41] S. Ishida, T. Masaki, S. Fujii, and S. Asano, Physica B **245**, 1 (1998).

[42] U. Geiersbach, A. Bergmann, and K. Westerholt, J. Magn. Magn. Mater. **240**, 546 (2002).

[43] Half-Heusler alloys: I. Galanakis, P.H. Dederichs, and N. Papanikolaou, arXiv:cond-mat/0203534; Full-Heusler alloys: I. Galanakis, P.H. Dederichs, and N. Papanikolaou, arXiv:cond-mat/0205129; Surfaces of Heusler alloys: I. Galanakis, arXiv:cond-mat/0204083; CrAs: I. Galanakis, arXiv:cond-mat/0203535.

[44] S.H. Vosko, L. Wilk, and N. Nusair, Can. J. Phys. **58**, 1200 (1980).

[45] P, Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964); W. Kohn and L.J. Sham, Phys. Rev. **140**, A1133 (1965).

[46] R. Zeller, P.H. Dederichs, B. Újfalussy, L. Szunyogh, and P. Weinberger Phys. Rev. B **52**, 8807 (1995).

[47] N. Papanikolaou, R. Zeller, and P.H. Dederichs, J. Phys.: Condens. Matter **14**, 2799 (2002).

[48] R. Zeller, Phys. Rev. B **55**, 9400 (1997); K. Wildberger, R. Zeller, and P.H. Dederichs, Phys. Rev. B **55**, 10074 (1997).

[49] R. Zeller, J. Deutz, and P.H. Dederichs, Sol. St. Comm. **44**. 993 (1982); K. Wildberger, P. Lang, R. Zeller, and P.H. Dederichs, Phys. Rev. B **52**, 11502 (1995).

[50] H.J. Monkhorst and J.D. Pack, Phys. Rev. B **13**, 5188 (1976).

[51] M.J. Otto, R.A.M. van Woerden, P.J. van der Valk, J. Wijngaard, C.F. van Bruggen, C. Haas, and K.H.J. Buschow, J. Phys.: Condens. Matter **1**, 2341 (1989); M.J. Otto, R.A.M. van Woerden, P.J. van der Valk, J. Wijngaard, C.F. van Bruggen, and C. Haas, J. Phys.: Condens. Matter **1**, 2351 (1989).

[52] J. Kübler, Physica B **127**, 257 (1984).

[53] M.V. Yablonskikh, V.I. Grebennikov, Yu.M. Yarmoshenko, E.Z. Kurmaev, S.M. Butorin, L.-C. Duda, C. Såthe, T. Kämbre, M. Magnuson, J. Nordgren, S. Plogmann, and M. Neumann, Solid State Commun. **117**, 79 (2001); M.V. Yablonskikh, Yu.M. Yarmoshenko, V.I. Grebennikov, E.Z. Kurmaev, S.M. Butorin, L.-C. Duda, J. Nordgren, S. Plogmann, and M. Neumann, Phys. Rev. B **63**, 235117 (2001).

[54] A. Kimura, S. Suga, T. Shishidou, S. Imada, T. Muro, S.Y. Park, T. Miyahara, T. Kaneko, T. Kanomata, Phys. Rev. B **56**, 6021 (1997).

[55] R.A. de Groot, A.M. van der Kraan, and K.H.J. Buschow, J. Magn. Magn. Mater. **61**, 330 (1986).

[56] D. Brown, M.D. Crapper, K.H. Bedwell, M.T. Butterfield, S.J. Guilfoyle, A.E.R. Malins, and M. Petty, Phys. Rev. B **57**, 1563 (1998).

[57] R.A. Dunlap and D.F. Jones, Phys. Rev. B **26**, 6013 (1982); S. Plogmann, T. Schlathölter, J. Braun, M. Neumann, Yu.M. Yarmoshenko, M.V. Yablonskikh, E.I. Shreder, E.Z. Kurmaev, A. Wrona, and A. Ślebarski, Phys. Rev. B **60**, 6428 (1999).

[58] D. Jung, H.-J. Koo, and M.-H. Whangbo, J. Mol. Struct. (Theochem) **527**, 113 (2000).

[59] J. Tobola, J. Pierre, S. Kaprzyk, R.V. Skolozdra, and M.A. Kouacou, J. Phys.: Condens. Matter **10**, 1013 (1998).

[60] L.P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. **50**, 58 (1936).

[61] P.G. van Engen, K.H.J. Buschow, and M. Erman, J. Magn. Magn. Mater. **30**, 374 (1983).

[62] W. Pendl Jr., R.N. Saxena, A.W. Carbonari, J. Mestnik Filho, and J. Schaff, J. Phys.: Condens. Matter **8**, 11317 (1996).

[63] Ye Feng, J.Y. Rhee, T.A. Wiener, D.W. Lynch, B.E. Hubbard, A.J. Sievers, D.L. Schlagel, T.A. Lograsson, and L.L. Miller, Phys. Rev. B **63**, 165109 (2001); C.S. Lue, J.H. Ross Jr., K.D.D. Rathnayaka, D.G. Naugle, S.Y. Wu and W.-H. Li, J. Phys.: Condens. Matter **13**, 1585 (2001); Y. Nishino, H. Kato, M. Kato, U. Mizutani, Phys. Rev. B **63**, 233303 (2001); A. Matsushita, T. Naka, Y. Takanao, T. Takeuchi, T. Shishido, and Y. Yamada, Phys. Rev. B **65**, 075204 (2002).

[64] T. Kanomata, M. Kikuchi, H. Yamauchi, and T. Kaneko, Jpn. J. Appl. Phys. **32** Suppl **32-33**, 292 (1993); M. Gotoh, M. Phashi, T. Kanomata, and Y. Yamaguchi, Physica B **213&214**, 306 (1995); S. Ishida, S. Kashiwagi, S. Fujii, and S. Asano, Physica B **210**, 140 (1995); .M. Pugacheva and A. Jezierski, J. Magn. Magn. Mater. **151**, 202 (1995)

[65] S. Jha, H.M. Seyoun, G.M. Julian, R.A. Dunlap, A. Vasquez, J.G.M. da Cunha, and S.M.M. Ramos, Phys. Rev. B **32**, 3279 (1985).

[66] C.N. Borca, T. Komesu, and P.A. Dowben, J. Electron Spectrosc. Relat. Phenom. **122**, 259 (2002).

[67] M. Shirai, Physica E **10**, 143 (2001).