Ψ_k Newsletter

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

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Contents

1 Editorial

The most important news is that recently the Psi-k Network member, Gerrit van der Laan from Daresbury Laboratory (UK), together with Paolo Carra (Grenoble) and Gisela Schütz (Würzburg), has received Europe's Most Prestigious Physics Prize, the Agilent Technologies Europhysics Award for the year 2000, for the **"pioneering work in establishing the field of magnetic X-ray dichroism".** Please see the **General News** section for more details on the physics background of this year's award. There also an up to date list of all recipients of this award is given. In the same section we publish very important details on the Psi-k 2000 Conference regarding registration, submission of abstracts, and above all the plenary talks, symposia and invited speakers. As usually, in this newsletter readers can find reports on collaborative visits and visits to conferences/workshops, conferenc/workshop announcements and a number of abstracts of newly submitted papers. In particular, in the section dedicated to the **TMR2 Network** we have the second annual report on the last year's activities of this network. In the **General Job Announcements** section there are several announcements of available positions. In the section **Presenting Other Initiatives** K. Parlinski (Cracov, Poland) writes about a computer code called **PHONON**. The scientific highlight of this newsletter is by Ph. Kurz, G. Bihlmayer, F. Förster, S. Blügel (*Jülich*) and L. Nordström (*Uppsala*) on **"FLAPW goes Non-collinear"**.

Please check the table of contents for further details.

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

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

The above contains pointers to home pages of some of the members of our electronic structure community. If you maintain a home page on your activities we will be happy to include a pointer from the *Networks'* home page to your home page.

Please note that the home page of the Psi-k Networks has recently been updated. It contains useful information regarding funding of workshops and collaborative visits within the ESF Programme. Its major new feature is a separate highlight section which contains all highlight articles of the Newsletters published so far.

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

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

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

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2 General News

2.1 Network Member shares Hewlett Packard Europhysics Award

LATEST NEWS

Network Member shares Europe's Most Prestigious Physics Prize

"Agilent Technologies Europhysics Award for the Discovery of Magnetic X-ray Dichroism"

Paolo Carra (ESRF, Grenoble, France), **Gerrit van der Laan** (Daresbury Laboratory, Warrington, UK) and **Gisela Schütz** (Institute of Physics, Würzburg, Germany) have won the Agilent Technologies Europhysics Award for the year 2000 for their

"Pioneering work in establishing the field of magnetic X-ray dichroism".

The award is given for "work leading to advances in the fields of electronic, electrical and materials engineering which represents scientific excellence".

The award ceremony took place on March 17 during the EPS Condensed Matter General Conference in Montreux, Switzerland. The Agilent Technologies Europhysics Award was formerly known as the Hewlett Packard Europhysics Award. Due to the recent split by Hewlett Packard into two separate companies (Hewlett Packard for the development sale of computer equipment and Agilent Technologies for the development and sale of equipment for systems and measures), this prestigious award is now given by Agilent Technologies. The prize is awarded every year for recent work by one or more individuals in the area of physics of condensed matter, specifically work leading to advances in the fields of electronic, electrical and materials engineering which represents scientific excellence. A complete list of prize winners over the years is given below. This list contains no less than seven Nobel prize laureates, namely von Klitzing (Physics, 1985), Binnig and Rohrer (Physics, 1986), Bednorz and Müller (Physics, 1987), Kroto and Smalley (Chemistry, 1996).

Magnetic X-ray dichroism (MXD) is considered as one of the most important discoveries in the field of magnetism in the last decennial. Sum rules allow to separate the spin and orbital parts of the magnetic moment. They can be used to measure independently the orbital moment providing a useful insight into the microscopic origin of anisotropic magnetic properties, such as

the magnetocrystalline effect, easy direction of magnetization, magnetostriction and coercivity of magnetic materials. The surface sensitivity combined with the element and site specificity of the technique make it immensely valuable in the study of magnetic thin films and multilayers. The interesting special magnetic properties characteristic of thin films derive from modifications in symmetry and coordination of the atoms primarily at the surface and interfaces. Materials with enhanced spin and orbital moments, perpendicular anisotropy and antiferromagnetic coupling between ferromagnetic layers across a non-magnetic spacer can all now be prepared - the latter two types of materials are of great interest to the magnetic recording industry. Determination of the polarization of a non-magnetic metal at an interface with a ferromagnetic layer provides a useful insight into the coupling mechanism in such materials. An important part of the pioneering work in the field of MXD has been done by Theo Thole, who died on July 4th 1996 after a fatal fall down the stairs at his home. [1] Would he still have been alive, he certainly would have been sharing the Agilent award. A short - and far from exhaustive - history of MXD is presented below.

In 1985 Theo Thole, Gerrit van der Laan, and George Sawatzky [2] from the Rijks University Groningen (NL) predicted a strong magnetic dichroism in the $M_{4,5}$ X-ray absorption spectra of magnetic rare-earth materials, for which they calculated the temperature and polarization dependence. A year later this MXD effect was confirmed experimentally by van der Laan et al. [3]. Using linearly polarized soft X-rays from the ACO storage ring at Orsay near Paris and total electron yield detection, the Tb $M_{4,5}$ absorption edge of terbium iron garnet showed the predicted polarization and temperature dependence. The next year Gisela Schütz et al. [4] performed measurements using X-ray transition at the K edge of iron with circularly polarized X-rays, where the asymmetry in absorption is in the order of 10^{-4}. This was shortly followed by the observation of magnetic EXAFS. [5] A theoretical description for the XMCD at the Fe K absorption edge was given by Ebert et al. [6] using a spin-polarized version of relativistic multiple scattering theory with relativistic effects and spin polarization treated on equal footing. This was soon also extended to include the X-ray magneto-optical Kerr effect. [7]

In 1990 Chen et al. [8] observed a large magnetic dichroism at the $L_{2,3}$ edge of nickel metal. Also cobalt and iron were showing huge effects, which rapidly brought forward the study of magnetic $3d$ transition metals, which are of technological interest. Full multiplet calculations for $3d$ transition metal $L_{2,3}$ edges by Thole and van der Laan [9] were confirmed by several measurements on transition metal oxides. First considered as a rather exotic technique, MXD has now grown out as an important measurement technique for local magnetic moments. Dedicated beamlines and insertion devices for polarized X-rays were constructed at all synchrotron radiation facilities worldwide supporting extensive research programmes.

MXD can be explained by electric multipole transitions from the core state to unoccupied valence states in combination with the Pauli exclusion principle. In 1988 Thole and van der Laan [10,11] presented a general analysis to explain the systematic trends observed in the branching ratio of the $L_{2,3}$ edges in $3d$ transition metals and the $M_{4,5}$ edges in rare earth systems. Using angular momentum algebra they showed that the branching ratio of the isotropic spectrum is proportional to the angular part of the spin-orbit operator in the ground state. In 1992, Thole, Carra, Sette, and van der Laan [12] derived a further sum rule showing that the X-ray magnetic circular dichroism signal integrated over the entire absorption edge is proportional

to the orbital part of the magnetic moment. An additional sum rule was derived by Carra, Thole, Altarelli, and Wang [13], establishing the relation between the effective spin magnetic moment and the weighted difference in intensity over the two spin-orbit split edges. These sum rules have been confirmed by Wu and Freeman [14] and others using the thin film full potential linearized augmented plane wave energy band method and a tight binding analysis for Fe, Co and Ni metal. Carra et al. [15] extended these sum rules to electric multipole transitions. Sum rules in jj coupled operators were derived by van der Laan [16], who also showed that for metallic 3d transition metal systems the magnetocrystalline anisotropy energy is directly related to the anisotropic part of the spin-orbit interaction. [17] The expectation value of the spin-orbit interaction can be obtained using the sum rule for X-ray magnetic linear dichroism.

XMCD in transverse geometry, i.e. with the applied magnetic field perpendicular to the light helicity vector, gives the possibility to determine, element-specifically, the easy direction of magnetization. This was demonstrated by studying the changes in the magnetocrystalline anisotropy that occur when a 3 ML Co film was deposited onto a 33 ML thick Ni layer on Cu, inducing a spin reorientation from perpendicular to in-plane. [18]

Sum rules for X-ray magnetic scattering were derived by Luo, Trammell, and Hannon [19]. Circular dichroism in X-ray resonant magnetic scattering can be used to obtain the magnetization profile of magnetic patterns in thin films by using circular dichroism to recover the phase relation in X-ray resonant magnetic scattering. This has been demonstrated for single-crystalline FePd layers with striped magnetic domain pattern providing unambiguous evidence for the presence of magnetic flux closure domains. [20]

Magnetic dichroism is also present in core level and valence band photoemission. When the emitted photoelectron has no interaction with the system left behind, the dichroism is due to the angular dependent part of the electrostatic interaction between the core hole and localized valence electrons [21]. The general theory for dichroism in photoemission has been developed by Thole and van der Laan and is described in a series of four papers. [22] In Paper I the authors discuss the origin of the spin polarization and magnetic dichroism. The different ways to orient the polarizations of the magnetization, electric vector of the light and the spin of the photoelectron allow measurements of different kinds of correlations between the corresponding atomic properties: the valence spin, core hole orbital momentum and core hole spin, respectively. Fundamental spectra can be defined as those linear combinations of the polarized spectra that are directly connected to physical properties. They are the natural quantities to obtain the information about the many-electron system contained in the spectrum. Magnetic dichroism in core level photoemission, which gives the alignment between the valence spin magnetic moment and the core hole orbital moment requires both spin-orbit and electrostatic interactions. Therefore, the strength of this alignment can be expressed in terms of the magnitude of these interactions. In Paper II it was shown that for the emission from an incompletely filled localized shell, such as the 4f shell in the rare earths, the integrated intensities of the magnetic circular dichroism and spin spectrum are proportional to the ground state orbital and spin magnetic moment, respectively. In Paper III the angular dependence of the polarized photoemission is treated. The geometry can be separated from the physical properties and the angular dependence provides a way to measure higher magnetic moments. The interference term between the $l-1$ and $l+1$ emission channels allows to measure the odd magnetic moments with linearly polarized light. In

angle integrated photoemission these magnetic moments can only be measured with circularly polarized light. Resonant photoemission is described in Paper IV with a discussion on core-hole polarization and a derivation of super sum rules.

Finally, to mention just one recent interesting development, the combination of high-resolution transmission X-ray microscopy based on the zone plate technique with X-ray magnetic circular dichroism, providing a huge contrast, is a new technique to image magnetic domain structures with a lateral spatial resolution down to 30 nm. [23]

The above gives only some of the highlights in the area of MXD and is by no means a complete overview. MXD is a rapidly expanding field and lots of new results can be expected in the forthcoming years.

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J. Phys. D: Appl. Phys. **31**, 649 (1998).

APPENDIX: COMPLETE LIST OF PRIZE WINNERS OVER THE YEARS

2000, Montreux,
P. Carra (I), G. van der Laan (NL), G. Schuetz (D),
For Pioneering Work in Establishing the Field of Magnetic X-ray Dichroism.

1999, London,
C. Glallti (F), M. Reznikov (IS),
For Developing Novel Techniques for Noise Measurements in Solids Leading to Experimental Observation of Carriers with a Fractional Charge.

1998, Grenoble,
M. T. Rice,
For Original Contributions to the Theory of Strongly Correlated Electron Systems.

1997, Leuven,
A. Fert (F), P. Gruenberg (D), S. S. P. Parkin (GB),
For Discovery and Contribution to the Understanding of the Giant Magnetoresistance Effect in Transition-Metal Multilayers and for Demonstrations of its Potential for Technological Applications.

1996, Stresa,
R.H. Friend,
Pioneering work on Semiconducting Organic Polymer Materials and Demonstrating of an Organic Light Emitting Diode.

1995, Telford,
Yakir Aharonov (IL), Michael V. Berry (GB),
For Introduction Fundamental Concepts in Physics that have profound Impact on Condensed Matter Science.

1994, Madrid,
D.R. Huffman (USA) , W. Kraetschmer (D), H.W. Kroto (GB), R.E. Smalley (USA),
New Molecular Forms of Carbon and their Production in the Solid State.

1993, Regensburg,
B.L. Altshuler (RU), A.G. Aronov (RU), D.E. Khmelnitskii (RU), A.I. Larkin (RU), B. Spivak (RU),
Theoretical Work on Coherent Phenomena in disordered Conductors.

1992, Prague,
G. Ertl (D), H. Ibach (D), J. Peter Toennies (D),
Pioneering Studies of Surface Structures, Dynamics and Reactions through the Development of Novel Experimental Methods.

1991, Exeter,
K. Bechgaard (DK), D. Jerome (F),
For the Synthesis of a New Class of Organic Metals and the Discovery of their Superconductivity and Novel Magnetic Properties.

1990, Amsterdam,
R. Car (I), M. Parrinello (I),
A Novel and Powerful Method for the ab-initio Calculation of Molecular Dynamics.

1989, Nice,
F. Steglich (D), H.-R. Ott (CH), G.G. Lonzarich (GB),
Pioneering Investigations of Heavy-Fermion Metals.

1988, Budapest,
J.G. Bednorz (D), K.A. Müller (CH),
Discovery of High-Temperature Superconductivity.

1987, Helsinki,
I.K. Yanson (USSR),
Point-Contact Spectroscopy in Metals.

1986, Stockholm,
F. Mezei (H),
Neutron Spin Echo Spectroscopy.

1985, Berlin,
J. Als-Nielsen (DK), M. Pepper (GB),
The Experimental Study of Low Dimensional Physics.

1984, Prague,
G.K. Binnig (D), H. Rohrer (CH),
For building the Scanning Tunnelling Microscope.

1983, Lausanne,
A.F. Silvera (NL),
Atomic and Solid Hydrogen.

1982, Manchester,
K. von Klitzing (D),
Experimental Demonstration of the Quantized Hall Resistance.

1980, Leeds,
O.K. Andersen (DK), A.R. Miedema (NL),
Original Methods for the Calculation of the Electronic Properties of Materials.

1979, Paris,
E.A. Ash (GB), J.H. Collins (GB), Y.V. Gulaev (USSR), K.A. Ingebrigtsen (N), E.G.S. Paige

(GB),
The Physical Principles of Surface Acoustic Wave Devices.

1978, York,
Z.I. Alferov (USSR),
Heterojunctions.

1977, Leeds,
W.E. Spear (GB),
Amorphous Silicon Devices.

1976, Heidelberg,
W. Helfrich (D),
Contributions to the Physics of Liquid Crystals.

1975, Bucharest,
V.S. Bagaev (USSR), L.V. Keldysh (USSR), J.E. Pokrovsky (USSR), M. Voos (F),
The Condensation of Excitons.

2.2 Psi-k 2000 Conference

"Ab Initio (from Electronic Structure) Calculations of Complex Proceses in Materials"

Schwäbisch Gmünd, 22-26 August, 2000

Conference Programme

The Programme Committee decided to reserve around 110 slots for 30 minute invited talks, around 130 slots for 15 minute contributed talks and 4 slots for 50 minute plenary talks. We shall also hold 2 poster sessions. Details of the programme (provisional speakers, etc.) are given below and can also be found on our Web site:

http://psi-k.dl.ac.uk/psi-k2000

The site also contains information about contributing papers, registration and accommodation, and below we highlight a few points on each topic.

Plenary talks, symposia and invited speakers

Plenary talks

Hardy Gross	New Directions in DFT
Norton Lang	DFT Studies in Molecular Electronics
Peter Levy	Magnetotransport in Multilayered Structures
Matthias Scheffler	The cutting edge: surfaces and their role in materials' properties

Symposium on "Bandstructure Methods"

O.K. Andersen	NMTOs
P. Dederichs	Conceptual improvements of the KKR method
E. Krasovskii	Electronic structure of bulk and semi-infinite crystals by the extended LAPW-kp method
N. Marzari	Localized Wannier functions in extended systems: theory and applications
T. Saha	Tight-Binding modelling and generation of first-principles Wannier-like orbitals using the new NMTO scheme
H. Skriver	Exact MT orbitals in the spherical cell approximation

Symposium on "Correlated systems"

S. Ezhov	Orbital occupation, local spin and exchange interactions in V2O3
A. Georges	Introduction to Dynamical Mean Field Theory and its possible use in realistic calculations
O. Gunnarsson	Resistivity of alkali-doped fullerenes: Lack of saturation at high temperatures
A. Liechtenstein	Beyond LDA
A. Mookerjee	Response functions and the recursion method
W.E. Pickett	Coexistence of High-Temperature Superconductivity and Magnetism: $RuSr_2GdCu_2O_8$
I. Solovyev	Aspects of charge, spin and orbital ordering in manganites

Symposium on "DFT"

R. Resta	Macroscopic polarisation and electron localisation in extended systems
L. Vitos	Kinetic and exchange functionals in the local Airy gas approximation

Symposium on "Excited States/Quasiparticles"

S. Louie*	Ab initio optical absorption and quasi particle spectra
L. Reining	Application of Greens function methods to calculation of excited states
A. Rubio	Lifetimes of hot electrons in metals
R. Del Sole	Ab initio calculation of optical properties of surfaces
W. Wolf	Screened exchange FLAPW calculations of optical properties

Symposium on "f-Electron Systems"

M.S.S. Brooks	Relativistic effects in f-electron systems
L. Nordström	Magnetism of the rare earth from first principles calculations
A. Svane	Self-Interaction Corrected Electronic Structure of Lanthanides and Actinides

Symposium on "Interfaces"

S. Koestlmeier	Ab-initio Investigation of Metal/Ceramic Bonding: Metal/Spinel Interfaces
A. Pasquarello	Silicon and its Oxide
W. Sigle(*)	To be announced

Symposium on "Large Systems/O(N)"

D. Bowler	CONQUEST: codes and applications
L. Colombo	To be announced
S. Goedecker	Linear scaling methods for electronic structure
P. Ordejon	Applications of SIESTA
D. Pettifor	Bond-order potentials: bridging the electronic to atomistic modelling hierarchies

Symposium on "Magnetism"

I. Abrikosov	Understanding the INVAR effect in Fe-Ni alloys
S. Baroni	Magnons in real materials from a generalized adiabatic decoupling scheme
S. Blügel	Magnetic phenomena at surfaces
J. Staunton	Dynamical spin susceptibility of alloys
L. Udvardi	Structure of Bloch walls: Heisenberg model vs. RSP calculations

Symposium on "Magnetoelectronics"

A. Barthelemy(*)	To be announced
J. Kudrnovsky	Ab initio theory of transport
I. Mazin	Is spin polarization a measurable quantity?
I. Mertig	Theory of GMR
N. Papanikolaou	Spin-dependent tunneling in metal-insutaltor junctions
E. Tsymbal	Spin-dependent tunneling

Symposium on "Materials Science"

G. Bihlmayer	The FLAPW method applied to complex magnetic systems
N.E. Christensen	New High-Pressure Phases in Alkali Metals and group IV Semiconductors
Z. Fang	Applications of ultrasoft pseudopotentials to 3d and 4d transition metal oxides
K. Fichthorn	Island nucleation in thin film epitaxy - a multiscale study
M. Gillan	How to find the chemical composition of the Earth's core using DFT
O. Jepsen	High pressure phases
G. Kresse	Fast all-electron ab-initio molecular dynamics
R. Martonak	Ab-initio molecular dynamics with a pressure reservoir: simulation of pressure-induced transformations in silicon clusters

Symposium on "Molecular and Biological Systems"

E. Artacho	Large scale calculations on DNA and proteins
P. Carloni	Drug-target interactions in anti-AIDS therapy: an ab initio approach
B. Lesyng	Mesoscopic Poisson-Boltzmann and Quantum-Classical Studies of Enzymatic Reactions
C. Rovira	Active centre in oxygen-carrying proteins
U. Roethlisberger	First-Principles Modeling of Enzymes
M. Segall	Biological applications of the CP method

Symposium on "Nanostructures and Quantum-dots"

M. Nardelli	Theory of electronic and transport properties of carbon nanotubes
D. Portal-Sanchez	Monoatomic gold wires
T. Todorov	Current-induced mechanical effects in atomic-scale conductors
A. Williamson	Calculations of multiple excitons in InAs quantum dots

Symposium on "Optimized Effective Potential"

E. Engel	Description of dispersion forces with implicit density functionals
A. Goerling	Advances in DFT by treating exchange exactly
M. Seidl	Strong-interaction limit of DFT: its simplicity and its relevance for electron systems

Symposium on "Polymers and Optoelectronics"

W. Barford	Conjugated Polymers
M. Cote	New polymers for optoelectronic applications
B. Delley	Structural switching in molecular complexes
I. Frank	Chemical reaction induced by mechanical stress: ab-initio simulations
E. Molinari	Excitons in polymer chains and crystals: an ab initio approach
W. Weiss	Screened exchange FLAPW calculations of optical properties

Symposium on "Quantum Monte Carlo"

M. Caffarel	New Developments in Quantum Monte Carlo calculations of observables
C. Filippi	Constructing optimal orbitals for QMC
R. Needs	Accurate QMC calculations for ground and excited states
S. Sorella	Strongly correlated electrons and QMC

Symposium on "Semiconductors"

P. Bloechl	On the calculations of defects in silica
M. Hierlemann(*)	To be announced
P. Kratzer	From DFT studies to growth simulations: Modeling molecular beam epitaxy of arsenide compound semiconductors
J. Ortega	Electron correlation effects and dynamical fluctuations at semiconductor surfaces: Sn/Si(111) and SN/Ge(111)
M. Pesola	Oxygen-related Defects in Si and GaAs
K. Schroeder	Theory of surfactant-mediated growth
C. Van de Walle	Properties of GaN surfaces: the role of H

Symposium on "Superconductivity"

J.F. Annett	Exotic superconductors
K. Capelle	Relativistic effects and dichroism in superconductors
E. Pavarini	Hyperfine fields in cuprate superconductors
D. Singh	Is singlet and triplet superconductivity incompatible?
Z. Szotek	Quasiparticles in d-wave superconductors

Symposium on "Surfaces"

A. Alavi	Chemistry at metal surfaces from density-functional theory: successes, failures and challenges
A. Bogicevic	Atom dynamics and diffusion on surfaces
V. Fiorentini	To be announced
J. Kollar	Stability of metal surfaces: Surface, step and kink formation energies
Y. Morikawa	Ab initio study of methanol synthesis over Zn-deposited Cu surfaces
J. Nørskov	Catalysis from first principles
C. Stampfl	Ab initio modelling of T-programmed desorption of molecules from metallic surfaces
H. Toalhout	Periodic trends and synergy effects in hydrodesulfurization catalysts: recent findings based on electronic structure calculations

Symposium on "Spectroscopies"

M. Alouani	Calculated Magnetic X-ray circular dichroism of binary alloys
S. Crampin	Calculations of second harmonic generation from magnetic interfaces
K. Karlsson	Cuprate core-level line shapes for different Cu-O networks
N. Lorente	First principles calculations of single molecule vibrational spectroscopy and microscopy
A. Paxton	Near edge structure in energy-loss spectroscopy of transition metal nitrides: some many electron and magnetic effects using density functional theory

J. Redinger	First-Principles Simulation of Scanning Tunneling Microscopy and Spectroscopy
G. van der Laan	Configuration interaction and correlation in magnetic 3d metals

(*) To be confirmed

Contributed Papers

The official call for contributed papers will begin on April 1, 2000 and we will be asking you to submit these contributions via the web site. You will be asked to state whether you would prefer to give a talk or present a poster, and we will do our best to arrange the schedule accordingly. Our policy is to try to accept one contribution from each participant in one form or another.

Registration

Registration will also begin, via the web site, on April 1, 2000. We expect most EU participants, contributing a talk or a poster, to be eligible for funding by one of the four Networks (please see below for details), and the web site will very soon provide information (eligibility, financial arrangements etc.) on this. We would strongly encourage you to read that information and the information below to establish your funding situation as soon as possible. If you have any queries or uncertainties about your eligibility for Network funding, please contact Walter Temmerman at Daresbury Laboratory (W.M.Temmerman@dl.ac.uk), who will be able to clarify and help.

Conference Fee

Please note that except for the plenary and invited speakers, all participants will be asked to pay the conference fee of 160 EURO at the early registration to the conference or 250 EURO at the late registration. However, those who will be awarded funding to attend the conference will get their conference fee refunded at the later stage.

Financial Support

Financial support may only be available to those EU participants who will offer to present a contribution (talk or poster) at the Conference. An application for funding should be directed to the national leaders of the nodes (partners) of the relevant TMR networks or the ESF programme involved in the organization of the Conference.

Specifically:

- If you belong to one of the research teams of the TMR Network on 'Ab initio calculations of magnetic properties of surfaces, interfaces and multilayers' (TMR1), i.e. if you are associated with one of the following nodes whose leaders are: Peter Weinberger (Austria), Hugues Dreyssé (France), Peter Dederichs (Germany), Börje Johansson (Sweden), Paul

Kelly (The Netherlands) and Walter Temmerman (UK), and the subject matter of your contribution concerns 'Interface Magnetism', then your costs, if approved, may be partially met by the relevant node. If this applies to you please contact the above mentioned node leaders.

- If you belong to one of the research teams of the TMR Network on 'Electronic structure calculations of materials properties and processes for industry and basic science' (TMR2), and the subject matter of your contribution is relevant to, and approved by, one of the nodes in this TMR Network, then your costs may partially be met by the Daresbury node (contact Walter Temmerman for details).

- If you do not fall in any of the two above categories, but your Institution is in one of the following countries: Austria, Belgium, Czech Republic, Denmark, Finland, France, Germany, Hungary, Ireland, Italy, Poland, Portugal, Slovenia, Spain, Sweden, Switzerland, United Kingdom, then your costs, if approved, may be partially met by the ESF programme STRUC (contact Walter Temmerman for details).

- If you belong to one of the research teams of the RTN Network on 'Computational Magnetoelectronics' and the subject matter of your contribution concerns Computational Magnetoelectronics, then your costs, if approved, may be partially met by the relevant national node. If this applies to you please contact for Austria: Peter Weinberger, for France: Albert Fert, for Germany: Peter Dederichs or Patrick Bruno, for Sweden: Börje Johansson, for The Netherlands: Paul Kelly, for Hungary: Janos Kollar, for the Czech Republic: Ilja Turek, for the US: Peter Levy and for the UK: Walter Temmerman.

- EU funds are available to support a limited number of young participants from Greece, Spain, Italy and Portugal. Please apply to Walter Temmerman for details.

Unfortunately, the EU and their INCO programme **has no funding** for the participation of other Eastern Europeans (Russia, Ukraine, etc.).

We are not in a position to provide funding for participants coming from non-European Institutions and these participants are advised to contact the appropriate member of the International Advisory Board if they request funding.

Accommodation

You need to book your accommodation directly through the Tourist Bureau in Schwäbisch Gmünd. The web site contains (in the page on Registration) an accommodation booking form for you to print off, complete and send to the Tourist Bureau.

Finally, we hope that our web site is proving as useful to you as it is to us. If you have any difficulty in using it, please contact us here at Daresbury straight away. Please consult the site frequently - it is a dynamical object!

3 News from the TMR1 Network "Interface Magnetism"

3.1 Workshop/Conference Announcements

3.1.1 Symposium on Spin-Electronics

3-6 July 2000 in Halle, Germany

`http://www.mpi-halle.de/~sse2000/`

Scope

This International Symposium will be organized in Halle by the Max-Planck-Institut für Mikrostrukturphysik and should bring together scientists active in the field of spin-electronics and spin-dynamics in order to discuss the latest experimental and theoretical developments, as well as technological applications. The subtopics will cover various aspects of spin-dependent transport, electronics and optics.

Timetable

February 29, 2000	Abstract submission deadline
April 22, 2000	Notification about acceptance and session assignment of the abstract
April 30, 2000	Deadline for early registration

Invited Speakers

D.D. Awschalom (*Santa Barbara*)	E. Beaurepaire (*Strasbourg*)
R.A. Buhrman (*Ithaca*)	J. Byers (*Washington*)
M. Johnson (*Washington*)	D. Loss (*Basel*)
S. Maekawa (*Sendai*)	L. Molenkamp (*Würzburg*)
S. Ogawa (*Hatoyama*)	H. Ohno (*Sendai*)
S.S.P. Parkin (*Almaden*)	J.M. de Teresa (*Orsay*)

Internet site

For details and registration to the Symposium please see the above web site.

3.2 Reports on Visits to Conferences/Workshops

Report on Two Conference Visits:

"Gordon Conference on Magnetic Nanostructures"
Ventura, CA, February 13-18, 2000
and
"International Symposium on Nanoscale Magnetism and Transport"
Sendai, Japan, March 8-10, 2000

The Gordon Conference was attended by about 130 people, mostly from the USA and Europe, the conference in Sendai by about 300 participants, of which 54 were "foreigners". Both conferences were very exciting and gave a representative cross section of the international activities in Nanoscale Magnetism. In short, magnetism is booming and the pace of progress is accelerating. It is fascinating to see the progress in industry in building prototypes of magnetic random access memories (MRAM), about which S. Parkin (IBM), S. Tehrani (Motorola) and P.P. Freitas (Lissabon) reported in Sendai. However other applications in Spin-Optoelectronics (K. Ando) and magnetic logic devices (G.A. Prinz) seem to be feasible in the future. For tunneling magnetoresistance there were very nice theory contributions by P.M. Levy, I.I. Oleinik, S. Maekawa and others, but the understanding is still underdeveloped and a lot remains to be done. Let us here shortly sketch some other highlights:

- The spin polarized STM has made it: There were beautiful experimental papers by J. Kirschner and R. Wiesendanger, so that in the future many more contributions in surface magnetism are to be expected.
- The spin-injection from dilute magnetic semiconductors (DMS) into normal semiconductors has been proven. Except for the paper of Akai (PRL(1998)) there is, however, practically no theoretical work for understanding the ferromagnetism of these systems (like $Ga_{1-x}Mn_xAs$).
- There were very nice GMR-contributions from our network (C. Blaas, P. Kelly, I. Mertig, P. Bruno). But as a whole the GMR activities are leveling off.
- Exchange-Biasing is an old subject, but rather purely understood. Also here more theory contributions would be helpful.
- There was a nice paper by R. A. Buhrman on the determination of the transmission coefficients through ferromagnetic layers by Andreev reflection.

The next Gordon conference will take place in 2002, presumably in Italy (Chairman R. J. Celotta, Vice-chair P. Bruno).

One of us (P. H. D.) visited in addition the "International Workshop on First-Principles Simulations of Advanced Magnetic Materials" organized by T. Oguchi in Suwa, which was a good opportunity to hear more about the many Japanese activities in the field.

Peter H. Dederichs

Nikos Papanikolaou

4 News from the TMR2 Network

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

4.1 Workshop/Conference Announcements

4.1.1 BdG Workshop

The VI Bristol Workshop on the Bogoliubov-de Gennes Equations

Burwalls, Bristol, United Kingdom
April 14-16, 2000

Sponsors: The European Science Foundation (ESF), TMR2 (EU) Network, and the Computational Collaborative Project 9 (CCP9) (UK)

Organisers: J F Annett, K P Duncan, E K U Gross and B L Györffy

http://rogers.phy.bris.ac.uk/bdg6/index.html

Introduction

The aim of the workshop is to bring together various communities whose work involves the Bogoliubov-de Gennes (or related) equations. Working in different fields such as superconductivity, superfluidity and nuclear physics, these groups do not cross paths in their daily research and have found this forum to exchange ideas very inspiring. The preliminary program of this year's workshop is:

Provisional Programme

April 14, Friday

20:00 Welcome and Buffet Dinner

April 15, Saturday

09:00-11:00	Density Functional Theory for Superconductors
	Gross, EKU (Würzburg + Bristol) Marques, M (Würzburg + Bristol)
	Capelle, K (San Carlos)
11:00-11:30	Coffee
11:30 -13:00	Exotic (non s-wave) Pairing
	Annett, J F (Bristol) Szotek, Z (Daresbury) Bertsch, G (Seatle)
	Monthoux, P (Cambridge)
13:00-14:00	Lunch
14:00-16:00	Mesoscopic Superconductivity
	Lambert, C (Lancaster) Büttiker, M (Geneva) Martin, A (Geneva)
	Zaikin (Moscow)
16:00-16:30	Coffee
16:30-18:30	Quasi-particles in Vortices and Interface
	Buzdin, A I (Bordeaux) Kümmel, R (Würzburg) Duncan, K P (Bristol)
	Volkov, A (Lancaster)
18:30-20:00	Dinner
20:00-21:00	Landau Levels or Bloch waves (?) in the Superconducting State
	Tesanovic

April 16, Sunday

09:00-10:00	Is the Repulsive-U Lattice Gas Superconducting?
	Jarrell, M (Cincinnati)
10:00-11:00	Preformed Pairs
	Quintanilla, J (Bristol) Wallington, J P (Leuven)
	Alexandrov, A S (Loughborough) Wilkin, N
11:00-11:30	Coffee
11:30-12:30	Disordered Superconductors
	Györffy, B L (Bristol) Litak, G (Lublin)

4.2 Annual Report of the TMR2 Network

Second Annual Report of TMR-Network: "Psi-k"

Electronic Structure Calculations of Materials Properties and Processes for Industry and Basic Sciences.

Reporting period: 01.03.99-29.02.00

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 scientific subprojects with 8 international teams in **DK**, **FR**, **GB** (2), **DE** (2), **AT** and **FI**. During the second year of operation the network has hired 4 more young researchers, while one has left for a permanent position. Hence, at present, 10 young researchers are financed by the TMR grant, and a total of 90.5 man months of PostDoc training has been delivered in the past year. Other principal Network activities include the organization of 3 workshops. The scientific program has grossly progressed as planned, as detailed below. We are currently seeking to enlarge the network with an additional partner, the Institut Superieur des Materiaux du Mans (ISMANS) in LeMans, France. This is motivated by the changes of staff at MSI, Paris, and the lack of scientific leadership of the **Surfaces** subproject.

The status of the scientific subprojects is as follows:

Surfaces

In March 1999 the network PostDoc (P. Gravil, **IE**) associated with the **Surfaces** subproject and based with MSI, Paris, accepted a permanent position within MSI, and a few months later the MSI scientist-in-charge (E. Wimmer) left the company for a position at an institution outside the network. After this happened the **Surfaces** subproject has been without scientific leadership and to a large extent inactive. As mentioned above, we are currently seeking to enlarge the network with a new partner, ISMANS, which is Prof. Wimmers new affiliation. ISMANS has agreed to become a member of the network and Prof. Wimmer to become the ISMANS scientist-in-charge. After this enlargement, hopefully the **Surfaces** subproject will be back on track. The new MSI scientist-in-charge is P. Gravil. Over the last year, very little progress has been made on the tasks 1A, 1B and 1C, but it seems still too early to change the workplan.

In a collaboration between TU-Wien and FHI-Berlin the role of rotational excitations in the dissociative adsorption of H_2 on Rh, Pd, and Ag (100) surfaces has been studied and published. The structure of the Al_2O_3 (0001) surface was studied by the Belfast group and results published.

f-electrons

The **f-electrons** subproject has a PostDoc based in Århus (L. Petit, **LU**, since September 99). The relativistic spin-polarized LMTO code with self-interaction corrections has been developed and task 2A thus completed. Applications to 5f systems (task 2B) has dominated the research since the PostDoc employment, with one publication submitted on the electronic structure of the actinide elements. The methodology correctly describes the 5f localization in elements beyond Pu as well as the trivalent-divalent switch between Cf and Es. Ongoing projects include monopnictides and monochalcogenides of Am and Pu, as well as laves phase actinide compounds. Thus task 2B is in full action and application to actinide systems will probably cover much of the activity for the remaining two years of the network operation. The strong collaboration between the Århus and Daresbury groups continues investigating both 4f and 5f systems, and the comparison of isoelectronic 4f and 5f compounds will be studied. Several publications on the application of the methodology to 4f systems (studies of rare earth elements and monosulphides and of Yb compounds) have been published and more projects are ongoing. Thus the study of 4f systems will continue to be a major activity of this subproject, although not foreseen in the work plan.

Task 2C, the implementation of full-potential total energy, has been initiated and first results are being evaluated in connection with the application of self-interaction corrections to high T_c superconductors.

Interfaces

Two network PostDocs (B. Montenari, **IT**, and since august 1999: A. Marmier, **FR**) are associated with the **Interfaces** subproject and based in Belfast. Dr. Marmier is working on ab-initio calculations (tasks 3A and 3C), while Dr. Montanari is developing the tight-binding approach for alumina (task 3B). This approach has been developed by the Belfast group and the succesful application to ZrO_2 has been published. The application to alumina(task 2B) has proved harder than expected, but progress has been made both in Belfast and in Stuttgart. In Belfast, attention has focussed on the effect of oxygen partial pressure on the equilibrium structure of interfaces. This was studied by an extension of calculations for the alumina surface and the Nb/alumina interface. In the case of Nb/alumina it was found that over most of the range of oxygen pressure an Al-terminated interface is thermodynamically more stable, although mechanically weaker. However, near the upper range of oxygen pressure (at which the oxide NbO begins to form) the energy difference is too small to resolve by the present methods. In Stuttgart, work has started on calculations for transition metals on $SrTiO_3$ (task 3D), and calculations for spinel-Al and spinel-Ag interfaces including authors from Stuttgart and Belfast have been submitted for publication.

Magnetism

Task 4A defines as one of the main goals of the **Magnetism** subproject the implementation of a noncollinear magnetic moment capability in the major electronic structure codes. Work at TU-Wien has completed the noncollinear versions of both k-space and r-space versions of LMTO and TB-LMTO codes and in the plane-wave-based projector-augmented-wave (PAW) code VASP. In the LMTO-codes noncollinearity is implemented, like in the noncollinear augmented spherical

wave (ASW) code of the Darmstadt group, in the form of an atomic-sphere-approximation (ASA - fixed quantization axis within each sphere), while in VASP the noncollinear version allows to treat the spin-density as a vector-field with a continuous variation of the direction and amplitude of the local magnetic moments. A similar fully unconstrained noncollinear version of the full-potential linearized augmented plane-wave (FLAPW) code FLEUR has been developed by the Jülich group, see also task 5B. This means that task 4A of the workplan has been essentially completed.

As part of task 4C, investigations of noncollinear magnetism in ordered intermetallic gamma-Fe-Mn compounds and disordered solid solutions have been performed. The striking result is that although canted noncollinear structures are found in the ordered compounds, the structural disorder in the solid solutions induces a collinear ordering of the magnetic moments. Noncollinear spin-structures have also been investigated in the closely related Mn-Ni compounds. Current work concerns the investigation of the noncollinear magnetic ground-state in alpha-Mn.

As part of task 4E, noncollinear spin structures in frustrated triangular antiferromagnetic layers (Mn and Cr monolayers on Cu(111) as well as freestanding monolayers) have been investigated, both in the ASA-LMTO and in the unconstrained PAW formalisms. This project is closely related to work of the Jülich group and task 5D. The formation of helical spin-structures has been investigated for Fe/Cr(100) superlattices.

The network PostDoc associated with the **Magnetism** subproject (D. Hobbs, **IE**, based in TU-Wien) has been involved in all of the above tasks, and several publications are in preparation.

In a collaboration between Helsinki and TU-Wien, the spontaneous magnetization of Al-nanowires on a NaCl-surface was studied.

LAPW

Three network PostDocs are associated with the **LAPW** subproject (G. Bihlmayer, **AT**, and S. Clarke, **UK**, in Jülich and G. Madsen, **DK**, since February 2000 at TU-Wien). As planned, the research activity of the **LAPW** subproject has focussed on the development of efficient FLAPW codes for the dynamics (Task 5A) and the application to problems related to the spin-polarized relativistic effects (Task 5B), such as the magnetic anisotropy, magneto-optics and non-collinear magnetism. Two codes are currently being developed, the WIEN99 code and the FLEUR code. In order to improve the efficiency of the codes and to learn from the different performances of the codes, we have set up a couple of benchmark problems (e.g. the (4x2)Cu(110) surface) which are treated by both codes. These tests will be continued into the third year. Performances of the codes are prepared to be published.

The capability of the spin-polarization part of the codes have been extended to treat non-collinear structures in real space and reciprocal space (spin spiral) (Jülich and Uppsala group). The directions of the magnetic moments within the sphere around an atom can be relaxed or can take arbitrary prescribed values with respect to neighboring atoms. The total energy is calculated within the formulation of the constraint density functional theory. The method to determine the ground-state orientation of the magnetic moments self-consistently has been implemented and explored. The two groups of Jülich and TU-Wien have implemented static, planar electric fields into the Wien99 and FLEUR codes. The TU-Wien group used the im-

plementation to investigate electron densities and internal strains due to the electric field in GaAs and to interprete synchrotron diffraction measurements (publication in preparation). The Jülich group investigated the properties of the Fe(001) surface, the results of which are being used to prepare a paper. The FLEUR code has also been used to investigate the results of the magneto-crystalline anisotropy, work which has resulted in a patent.

A joint activity of the groups in Graz and Uppsala is the calculation of electron-phonon coupling constants in metals. For that purpose, the changes in Hamilton matrix and overlap matrix due to displacements of atoms are necessary ingredients. Two different procedures have been tested: The required quantities have been obtained from (a) two self-consistent calculations, or (b) by use of the linear response method, which had been developed on basis of the WIEN97 code in Graz before. The results of both methods excellently agree for all test substances and phonon modes. The method is currently applied to study q-dependent electron-phonon coupling constants in superconducting materials. A publication is in preparation. Students from Uppsala have visited Graz for several times and further long-term visits are planned. A collaboration between Graz and the Århus group studies ferroelectricity in $SrBi_2Ta_2O_9$.

The code development concerning optical properties in presence of spin-orbit coupling has been finished in Graz. In that context, the optics package has been updated together with the TU-Wien group with magnetooptics beeing a new feature in the WIEN97 code.

After two years of code development (tasks 5A and 5B) this part of the project has essentially been accomplished, and future emphasis will be on applications (tasks 5C and 5D).

Excitations

Two network PostDocs are associated with the **Excitations** subproject, (J.-L. Muzos, **ES**, and since January 2000 J. J. Hogan-O'Neill, **UK**, both based with the Helsinki group). The focus has been to test different novel schemes to account for excitations beyond standard LDA, or GGA, description (task 6A). These are based in (1) alternative exchange-correlation functionals such as the screened exchange local density approximation (sx-LDA), and (2) application of time-dependent density functional theory (TD-LDA) to linear excitations.

The case (2) is a promising collaboration between Helsinki and Würzburg. The difficulties regarding the application of TD-LDA to extended insulating systems have been clarified. Standard exchange-correlation kernels such as adiabatic LDA or optimized-effective-potentials, would result in asymptotically vanishing corrections in the thermodynamic limit. On the other hand, the inclusion of macroscopic polarization effects into the theory provides finite corrections to the LDA gap excitations. At present, the only formulation avaliable is the inclusion of the current-density response function in the theory. Alternative formulations are pursued, leading to exchange-correlation kernels including the macroscopic polarization. This could also be done including in a semiempirical fashion the screening of the Coulomb interaction with the macroscopic dielectric constant. This might provide satisfactory results in calculations of vertical excitations for deep centers in semiconductors.

As part of task 6B of the workplan, optical transitions of oxygen centers in GaN have been studied, to be published soon. Task 6C is still at the preparatory stage.

Superconductivity

The strong collaboration between Würzburg, Daresbury and Bristol on ab-initio studies of superconductors continues. In Daresbury investigations of the quasiparticle spectra of YBCO in the superconducting state (task 7A) have been performed, with focus on the two components of the penetration depth tensors λ_a and λ_b, as functions of the temperature T and doping. Three separate points of physical interest are highlighted by our results: Firstly, we have presented further evidence in support of the experimental suggestion that the measured anisotropy of $\lambda_a(0)/\lambda_b(0) \sim 1.5$ implies significant superconducting condensate on the Cu-O chains in the a-b plane. Secondly we showed that the temperature dependence of the superfluid density, as represented by $\lambda_a^2(0)/\lambda_a^2(T)$ and $\lambda_b^2(0)/\lambda_b^2(T)$, is well described by the quasiparticles which also gave a good account of the photoemission experiments. Thirdly, our calculations reproduced the experimentally observed universality of the behavior of $\lambda_{\alpha\alpha}^2(0)/\lambda_{\alpha\alpha}^2(T)$ with respect to doping, indicating that this dependence, like that of T_c, is governed by the movement of the chemical potential ε_F with respect to a Van Hove singularity in the normal state electronic structure. With these results (which are currently being prepared for publication) the task 7A has been largely completed.

The Würzburg group in collaboration with Bristol has made considerable progress on the construction of first-principles functionals for the xc energy in the superconducting state (task 7B). In the first step, a universal LDA-type functional describing the purely electronic correlations in superconductors has been developed based on the homogeneous electron gas. In a second step, functionals describing the electron-phonon coupling have been derived. By putting both functionals together and solving the resulting gap equation, we have successfully calculated the critical temperatures of simple metals. The agreement of the calculated T_c's and the experimental numbers, being typically within a few percent, is very encouraging. The network PostDoc, (L. Fast, **SE**), has mostly been involved with this last part of the research program. This work has been submitted for publication.

A collaboration between the Graz and Uppsala groups has been established to study the structural phase diagram of Y-Ba-Cu-O superconductors. Effective interaction parameters of the oxygen ions within the basal plane of $YBa_2Cu_3O_{7-x}$ are obtained from total energy calculations for different configurations of oxygen ordering. These pair interactions parameters are used to study effects of temperature and oxygen concentration within the Monte-Carlo method. The stability of different Cu valencies in $YBa_2Cu_3O_n$ is studied in a collaboration between the Århus and Daresbury group.

Training and Dissemination

This subproject is concerned with training and dissemination (Tasks 8A, 8B and 8C). 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 group coordinates these activities, which involve all network partners.

During the reporting period, six Newsletters were published, in April, June, August, October,

December 1999 and February 2000. This Newsletter is e-mailed to more than 700 e-mail addresses and is also available on the home page of the TMR Network. Part of the newsletter is a scientific highlight section and this year five of these highlights were contributed by one of the present network subprojects. The Majordomo mailing lists and the psi-k www pages are kept up-to-date.

Three workshops have been organized in the past year.

The **LAPW** subproject organised a Hands-on workshop in the use of the LAPW methodology in Wien, (April 7-10 1999), teaching both basic principles and new developments.

A workshop entitled *Orbital and Spin Magnetism of Actinides* was organised by the **f-electrons** subproject and held in Daresbury (June 4-5, 1999). The purpose of the workshop was to convene experimental and theoretical researchers in actinide physics. The magnetism of 5f systems is less well understood than that of 3d and 4f systems. The strong spin-orbit interaction necessitates a relativistic approach, and electron correlation effects play a major role. On the experimental side it has recently become possible to determine element specific magnetic moments using neutron diffraction and x-ray scattering and absorption. The latter technique makes it even possible to separate the orbital and spin contribution to the total magnetic moment. The results are very interesting but difficult to reproduce with present state-of-art calculations.

A Hands-on Workshop on *Calculation of Materials Properties using Total Energy and Force Methods and ab initio Molecular Dynamics* on the basis of the FHI98md Computer code was organised in Trieste (9-18 August 1999). This 10-days course was directed by P. Kratzer from FHI-Berlin. Co-directors were J. Kohanoff (ICTP, Trieste), J. Neugebauer (FHI), and M. Scheffler (FHI). The workshop was concerned with detailed presentations on basic aspects of DFT, pseudopotential concepts, ab initio molecular dynamics, time-dependent DFT, and many-body schemes. In addition to the talks, there were practical, hands-on sessions, in which the use of the FHI98md computer code and the construction of pseudopotentials was taught. Because of the limited number of available terminals, the number of participants had to be limited to 80 people. However, 235 people had applied. Participants and tutors have written reports with their viewpoints concerning the activity and this can be found in Psi-k Newsletter # 35.

Good progress in the organisation of the Psi-k Conference (Task 8C) has been made. This Conference, Psi-k2000 will take place in Schwäbisch Gmünd on August 22-26, 2000. The programme committee of the Psi-k2000 Conference met in Paris on December 11, 1999. The selection of the invited speakers was made at that meeting. The invitations have gone out and most of the invited speakers have now accepted. The programme can be viewed on the Conference web-site given below.

The Third Management Board Meeting took place in Paris on October 23rd, 1999.

The network homepage address has changed to:

http://www.ifa.au.dk/~svane/tmr-psik.htm

which includes links to the newsletters.

The homepage of the Psi-k2000 conference is: **http://psi-k.dl.ac.uk/psi-k2000**

5 News from the ESF Programme

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

5.1 Workshop/Conference Announcements

5.1.1 Psi-k/ESF - CECAM Workshop

We announce the workshop on

"Catalysis from First Principles"

Lyon, July 5 - 8, 2000

sponsored by the Psi-k/ESF Network and CECAM

Participation is by invitation only. However, at this time please feel free to suggest invited speakers and/or participants (also yourself!!) by sending an e-mail to Matthias Scheffler (scheffler@fhi-berlin.mpg.de).

Organizers:

Jürgen Hafner
Jens Nørskov
Matthias Scheffler

Workshop Objective:

The objective of the meeting is to review the status of total-energy calculations as a basis for modeling and understanding of chemical reactions on solid surfaces. A strong focus will be placed on the prospects of calculational methods becoming a tool in the design of new catalysts. An additional objective is to bring together researchers from the electronic structure, the molecular-dynamics, the statistical physics community as well experimental surface-science and catalysis researchers from academia and industry.

For further details, please check here:

http://www.fhi-berlin.mpg.de/th/Meetings/Lyon2000/Lyon-1.html

5.1.2 Cagliari Workshop

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

X WORKSHOP ON
COMPUTATIONAL MATERIALS SCIENCE

7 - 12 September 2000
Tanka Village, Villasimius (CA), Sardinia, Italy

web page: http://www.dsf.unica.it/CMS2000
e-mail: workshop@dsf.unica.it

under the patronage of UNESCO

An international workshop on computational techniques and applications to materials science

VENUE: Tanka Village 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

SCHEDULE:

7 September:	ONLY arrivals
8 September:	full program (4 morning plus 2 afternoon lectures)
9 September:	full program plus poster session
10 September:	conference trip; panel discussion
11 September:	full program plus poster session
12 September:	morning session (4 lectures); departures

Transfer from Elmas airport to Tanka Village (∼1 hour) will be organized; we plan to set up a couple of buses on Septmber 7 at around 2 pm and 5 pm. Further details are or will be posted on our web site:

http://www.dsf.unica.it/CMS2000

INVITED SPEAKERS:

A. Baldereschi (EPFL, Switzerland)	(interfaces and contacts)
S. Baroni (SISSA, Italy)	(linear response and phonons)
(*)M. Cardona (MPI-FKF, Germany)	(semiconductors spectroscopy [exp.]
J. Frenken (Leiden)	(surface [exp.])
W. Kohn (UCSB, USA)	(DFT)
R. O. Jones (FZ Juelich, Germany)	(polymers and clusters)
U. Landman (Atlanta, USA)	(tribology, large scale simulations)
M. Parrinello (MPI-FKF, Germany)	(ab initio MD; ice, biosystems, etc.)
R. Resta (U Trieste, Italy)	(polarization and ferroelectricity)
M. Scheffler (FHI-MPG, Germany)	(theory of surfaces and catalysis)
(*)E. Tosatti (SISSA, Italy)	(high pressure physics, high-T surfaces)
A. Zunger (NREL, USA)	(alloys and nanostructures)

(*) not yet confirmed

For further details please contact V. Fiorentini or P. Ruggerone at workshop@dsf.unica.it.

Report on a Collaborative Visit of J. L. Mozos (Laboratory of Physics, Helsinki University of Technology) to Prof. E. K. U. Gross (University of Würzburg)

13 – 31 January, 2000

During my visit to Prof. E. K. U. Gross' group we discussed over the application of Time-Dependent Density Functional Theory (TD-DFT) to the calculation of excitations in extended insulating systems.

Specializing the TD-DFT to the linear response regime, it yields the corresponding linear excitations of the system. This has been applied to calculations for finite systems, with excellent quantitative results. However, standard exchange-correlation kernels, such as ALDA, result in asymptotically vanishing corrections in the thermodynamic limit for insulators. This problem is connected with the inclusion of the macroscopic polarization in the theory, which has a significant contribution to the long-wavelength optical response of the systems. On this regard, several ideas were already generated and tested during this visit in Würzburg by Prof. Gross' group members and collaborators.

We plan to apply this methodology to an ongoing project of calculation of vertical excitations in deep centers in semiconductors, carried out here in Helsinki.

I value very positively this visit and I am very grateful to the network for its support, which made it possible.

José-Luis Mozos

Report on a visit of Diemo Ködderitzsch (Halle/Saale, Germany) to Professor Walter Temmerman's group (Daresbury Laboratory, UK)

January 24 - February 4, 2000

During this visit to Daresbury Laboratory we continued our collaborative work which had been initiated at my previous visit in January, 1999.

One of the objectives of this visit was to discuss my recent results obtained in the examination of i) different magnetic structures of the transition-metal oxides NiO and CoO and ii) the properties of the surfaces of these materials as calculated by means of the self-interaction corrected LMTO-ASA code that I became familiar with during my previous stay at Daresbury Laboratory. This code implements the self–interaction correction (SIC) to the local density approximation in the framework of Density functional theory.

As our calculations for the bulk NiO and CoO reveal, in both cases the AF2 order is energetically favoured, followed by the ferromagnetic and the AF1 phases. For NiO this order stays the same in the model calculations for the (001) (1x1) surface which we have carried out using a supercell approach to describe the surface. So one step towards the description of the surface of the transition-metal oxides within the SIC formalism has been taken. From our findings we argue that the AF2 structure will be the favoured one for the substrate. Our next aim is to examine different magnetic couplings of the surface layers to the AF2 ordered substrate.

Another subject of our discussions was the description of bulk CoO and its magnetic properties in the experimentally observed body-centred tetragonal cell (resulting from a small crystallographic distortion of the cubic structure). By analyzing the bands obtained from the SIC calculations we want to get more insight into the origin of the insulating gap. In addition we want to study the effect of the magnetic structure on the formation of bands.

Finally, we have also discussed an implementation of the local self-interaction correction within the KKR bandstructure method. The idea is to formulate the SIC in terms of the phase shifts of the relevant lm channels. A KKR code has already been developed in the group of Prof. Walter Temmerman. As this code is adapted to a layer geometry it will be well suited for studying the electronic structure of surfaces.

Diemo Ködderitzsch

Report on a visit of Philippe Ghosez (Universite de Liege, Belgium) to CSIC in Barcelona (Spain)

February 29 - March 3, 2000

The objective of visiting Dr Pablo Ordejon at the CSIC in Barcelona was to explore the possibility of a collaboration to investigate the growth mechanisms and the properties of ferroelectric thin films using SIESTA, a local-orbilal order-N DFT code developped by the Spanish group.

The evolution of the ferroelectric properties when switching from bulk to thin films is since a long time a problem of fundamental interest. It became more recently a question of technological importance after the finding of the possibility of epitaxial growth of ferroelectric titanates on Silicon (001) surfaces, which has opened the way to the integration of these compounds in microelectronic devices (such as non-volatile memories). In this context, our interest includes: (i) The growth of thin films of ferroelectric oxides with perovskite structure on different substrates; (ii) The thickness dependence of the structural transitions in these materials as a function of temperature, pressure, electric field, etc.

During the stay, we first checked the accuracy of the SIESTA code in reproducing the ferroelectric instability of barium titanate, a prototype ferroelectric compound, and we then defined a strategy of collaboration. Preliminary results on barium titanate confirm that the local-orbital method yield accuracy comparable to that previously obtained with other DFT technics and is therefore suitable to tackle the problem of the ferroelectricity in this material. Our plans are to look first at free-standing slabs under zero-field electrical boundary conditions. This will give us access to the microscopic quantities (interatomic force constants, Born effective charges, dielectric constant) necessary for the construction of a model Hamiltonian, comparable to that recently proposed for $PbTiO_3$, and which allows to investigate the ferroelectric properties in temperature. In a second step, we will consider the case of thin films of barium titanate on different substrates and investigate the influence of the latter on the properties of the film.

Philippe GHOSEZ

6 General Workshop/Conference Announcements

6.1 International DFT Conference in Antwerp

Second Announcement of the International Conference on

Density Functional Theory and its Applications to Materials

University of Antwerp, Belgium

June 8 - 10, 2000

http://www.ruca.ua.ac.be/dft2000

Contributions

Applications are invited for the above International Conference. Any density functional studies relevant to materials science may be proposed, whether on three-dimensional materials (e.g. semiconductors and metallic alloys), or on low-dimensional systems (e.g. polymers or 2D electron gases in heterojunctions). Calculations on medium- or large-sized clusters will also be considered, if they clearly throw light on the understanding of bulk or surface properties of materials.

The following scientists havealready accepted the invitation to lecture:

N.W. Ashcroft (Cornell University, Ithaca, U.S.A.)
G.B. Bachelet (University of Rome, Italy)
A. Baldereschi (Swiss Federal Institute of Technology, Lausanne, Switzerland)
R. Car (Princeton University, U.S.A.)
T.C. Collins (Oklahoma State University, Stillwater, U.S.A.)
J.T. Devreese (University of Antwerp, Belgium)
R.W. Godby (University of York, U.K.)
E.K.U. Gross (University of Wurzburg, Germany)
O. Gunnarsson (Max-Planck Institute, Stuttgart, Germany)
J. Krieger (Brooklyn College of CUNY, U.S.A.)
J. Ladik (University of Erlangen, Germany)
M. Levy (Tulane University, U.S.A.)
S. Louie (University of California, Berkeley, U.S.A.)
N.H. March (University of Oxford, U.K. - presently at: University of Antwerp, Belgium)
J.L. Martins (INESC, Lisbon, Portugal)
J. Mintmire (Naval Research Laboratories, Washington, U.S.A.)

M. Payne (University of Cambridge, U.K.)
F. Peeters (University of Antwerp, Belgium)
J.P. Perdew (Tulane University, New Orleans, U.S.A.)
G. Straub (Los Alamos National Laboratory, U.S.A.)
D. Wallace (Los Alamos National Laboratory, U.S.A.)

Persons whose applications are accepted will be encouraged to offer one hour poster presentations during the meeting. All participants (maximum 150), except students, are required to pay a registration fee of 250 EURO/$ (10000 BEF), which gives entitlement to conference documentation and proceedings, coffee and lunch, transportation to lecture hall and social events. The student fee is 125 EURO/$ (5000 BEF).

For further information please contact: V.E. Van Doren, Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, tel. +32/3/2180317, fax +32/3/2180318, e-mail: density@ruca.ua.ac.be

7 General Job Announcements

Postdoctoral Position in Condensed Matter Theory
Max–Planck–Institute Halle

The Max-Planck-Institute of Microstructure Physics at Halle, Germany, has a **postdoctoral position in Condensed Matter Theory** available for up to two years. The candidate for this position will develop a many-body theory of **Femtosecond Spin-Dynamics** in thin magnetic films using non-perturbative methods. The theory envisages the laser control of magnetism. Experience with many-body techniques (exact diagonalization, quantum chemical methods, Green's function techniques) or optical control formalisms is required for this position. The annual gross salary of the position amounts to approx 35,000 Euros depending on age, experience, and marital status (BAT IIa according to German Salary Scale). The Max-Planck Society is an Affirmative Action/Equal Opportunity employer. Applications from women, minorities, and disabled persons are encouraged.

Candidates for the position, which is open to all nationalities, should send an application including a CV and the names of three references to:

Dr. W. Hübner,
Max-Planck-Institut für Mikrostrukturphysik Halle,
Weinberg 2, D – 06120 Halle,
Germany
Fax: +49-345-5511 223,
email:huebner@mpi-halle.de .

Professor of Computational Physics

Institute for Experimental Physics, Faculty of Sciences, University of Vienna

There is an opening for a professor of Computational Physics We look for a candidate with excellent scientific record in a field which emphasizes the great variety of methods and applications of Computational Physics at the Faculty of Sciences. The candidate will have to do research and teaching in the field, and will have to participate in the education of students majoring in Computational Physics. The candidate should have a "Habilitation" or an equivalent qualification, teaching experience, management of habilities, and a successful record in international research.

Further information about the institute can be found at:

http://www.exp.univie.ac.at

Applications should contain a curriculum vitae, the professional/scientific curriculum, publication list plus reprints of the five most important papers as well as a description of the teaching experience and current research projects. They should be received at the:

Dekanat der Naturwissenschaftlich-Mathematischen
Fakultat der Universitat Wien,
Dr. Karl Luegerring 1
A-1010 Wien - Austria

no later than April 15, 2000.

Female scientists are particularly encouraged to apply and will be given preference in case of equal qualification.

Enquiries from the Psi-k community can be directed to:

Prof. Juergen Hafner
Institut fuer Materialphysik and
Center for Computational Materials Science
Universitaet Wien
Sensengasse 8/12
A-1090 Wien, Austria

Tel.: +43-1-4277-51400
Fax : +43-1-4277-9514
Email: Juergen.Hafner@univie.ac.at

Postdoctoral Research Associate, Fixed term (3 years)

Imperial College London and Royal Institution of Great Britain

The Computational & Structural Chemistry Group, Department of Chemistry, Imperial College London and the Davy Faraday Laboratory of the Royal Institution of Great Britain seek a research scientist to join a three year project on the use of high performance computers for the simulation material properties. The project is part of an established national collaboration (the Materials Science Consortium) which has been at the forefront of exploiting massively parallel computers for the simulation of material properties. In addition to the application of both first principles and empirical modelling software to a number of problems in bulk and surface materials science there will be an opportunity to work on the development of software on state of the art computer facilities.

The successful candidate will have relevant experience in condensed matter physics or chemistry and a Ph.D. (or equivalent) in a relevant discipline. Experience of collaborative software development and/or high performance computing is also desirable.

Additional information is available from Professor N.M. Harrison (email n.harrison@dl.ac.uk) or Professor C.R.A Catlow (email richard@ri.ac.uk).

Applications, enclosing a c.v. and the names of two referees, should be sent to Professor Nicholas Harrison, Department of Chemistry, Imperial College London, London, SW7 2AY, U.K or Professor Richard Catlow, Davy Faraday Laboratory, The Royal Institution, 21 Albermarle Street, London, W1X 4BS.

Ab initio Theory of Photochemistry
Postdoctoral Fellowship and two Ph.D. Studentships

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (Germany)

The Theory Department of the Fritz-Haber-Institut in Berlin-Dahlem invites applications for a postdoctoral fellowship and a Ph.D. studentship in theoretical photochemistry. Photochemistry represents a rapidly growing, interdisciplinary field that aims at developing techniques for the external control of reaction dynamics through photon irradiation. A particularly high potential for future applications lies in reactions between molecules and surfaces, such as laser-induced desorption, which promises to soon become an efficient method for preparing surface microstructures as well as quantum-state selected molecules in the gas phase.

One **Postdoctoral Fellowship**, lasting for two years with the possibility of extension, will be funded as part of the EU Research Training Network "Nanoscale Photon Absorption and Spectroscopy with Electrons" (subject to successful contract negotiation). To be eligible candidates must be (i) aged 35 years or less, (ii) a citizen of a member state of the European Union or an associated state of the Fifth Framework Programme, excluding Germany, (iii) resident and working in Germany for no more than 12 months within the last two years. However, other suitably qualified candidates may be aided in obtaining external funding and are encouraged to apply. The value of **Ph.D. Studentships**, which extend over three years, complies with the rules of the Max Planck Society, but there is additional funding for travel and conference participation. All vacancies are immediately available.

The principal computational methods we employ to study the interaction of surfaces with admolecules are density-functional theory and many-body perturbation theory. Candidates should therefore have demonstrated expertise with first-principles electronic-structure/total-energy techniques. Applicants should send a curriculum vitae, highlighting their main achievements, together with a publication list to the address given below. Electronic applications are welcome, and reference letters will be given proper consideration. Please feel free to send an e-mail for informal inquiries.

Dr. Arno Schindlmayr
Fritz-Haber-Institut der Max-Planck-Gesellschaft
Faradayweg 4–6
14195 Berlin
Germany

E-mail: schindlmayr@fhi-berlin.mpg.de
Tel.: +49 (0)30 8413-4817
Fax: +49 (0)30 8413-4701

Further information about the group is available at http://www.fhi-berlin.mpg.de/th/th.html

Postdoctoral Position in Theoretical Surface Science
University College London

The Centre for Cosmic Chemistry and Physics at University College London (UCL) is carrying out a programme of theoretical and experimental investigations on the formation of astronomically important molecules via reactions on the surfaces of interstellar dust grains. The staff participating in the centre come from the Department of Physics and Astronomy, the Department of Chemistry, and the Department of Electrical Engineering. The centre is now expanding its activities following a recent major grant from the Leverhulme Trust.

We have a vacancy for a postdoctoral research fellow. The post is to work with Dr Andrew Fisher in the Department of Physics and Astronomy, carrying out Car-Parrinello calculations to give insight into the reaction pathways and mechanisms for the formation of molecules in star-forming regions of interstellar space. The work will involve collaboration with the theoretical chemistry group of Professor David Clary in the Department of Chemistry. In particular, we will simulate the formation of H_2O, NH_3 and CH_3OH on interstellar dust surfaces, complementing a programme of experimental research on these systems in the UCL Chemistry Department. Use will be made of the recently installed 48-processor Silicon Graphics Origin 2000 supercomputer in the UCL HiPerSPACE centre.

UCL is one of the largest and most research-active university institutions in the UK. It is the oldest and largest college of the University of London and is situated in the centre of the city close to the British Museum. The position will involve working in dynamic and active research groups and in collaboration with other members of the Centre. The appointments will be for up to three years, and the salary will be on the Research Fellow (1A) scale - currently 16286 to 24479 UK pounds per annum, plus 2134 pounds London weighting.

The initial closing date for applications is the end of March; thereafter we will continue to consider applications until the posts are filled. Applicants should have (or expect to obtain shortly) a PhD in a relevant discipline. Experience of atomistic simulations and/or electronic structure calculations would be an advantage.

Contact:

Dr Andrew Fisher: Telephone (+44) 20 7679 1378
mail to: andrew.fisher@ucl.ac.uk

For general information see:

http://www.ucl.ac.uk/ uccacdl/ (Centre for Cosmic Chemistry and Physics)
http://www.cmmp.ucl.ac.uk/ (Condensed Matter and Materials Physics)
http://calcium.chem.ucl.ac.uk/webstuff/index.html (Department of Chemistry)

The IHP (Innovations for High Performance microelectronics) invites applications for a Project Position in Interface Simulation

The IHP (Director Prof. Dr. A. Ourmazd) consists of approximately 180 research staff, primarily in the area of wireless communication and networking, including SiGe-based technologies, diagnostics and measurement techniques. We work in a multidisciplinary environment, spanning materials, process technology, circuits, and systems. The IHP is now housed in a state-of-the-art building 55 minutes from Berlin, with ultra-modern facilities.

The advertized position involves simulation of atomic and electronic structures of semiconductor/dielectric interfaces, and diffusion of dopant atoms in silicon. The successful candidate will most likely have a PhD in physics and documented experience in the development and application of atomistic computer programs. Experience in application of *ab initio* methods is an advantage. Responsibilities also include installation and management of appropriate computer programs.

The position will be filled as quickly as possible. The project position is for one year. Salary will be on the BAT scale.

Applications should be sent to:

Dr. Ch. Quick
IHP
Im Technologiepark 25
D-15236 Frankfurt (Oder)
Germany
Phone: +49 335 5625 330
Fax: +49 335 5625 447
E-mail: quick@ihp-ffo.de

Scientist Position

Theory and Modelization of Spin-Electronics Devices

Theory Department of the Max-Planck Institute of Microstructure Physics, Halle, Germany

A scientist position for 3 years is available in the Theory Department of the Max-Planck Institute of Microstructure Physics in Halle, Germany.

The successful candidate will be in charge of a project concerned with the theory and modelization of spin-electronic devices such as magnetic random access memories (M-RAM).

This work is part of the project "NanoMEM" funded by the European Commission within the "Information Societies Technology" Programme. The NanoMEM project is carried out jointly by several research groups from academia and industry from France, UK, and Germany, and aims at investigating new architectures of M-RAMs.

The role of the MPI in the NanoMEM project is to provide theoretical support on the physical problems encountered. The successful candidate will be in charge of carrying out model calculations of electric transport in magnetic tunnel junctions, as well as assisting the experimentalists in the conception and interpretation of their experiments. A strong background in quantum mechanics, statistical physics, solid state physics and magnetism, as well as experience in computer programming, are required. As well important are a good knowledge of the particular field of spin-electronics and a strong motivation for working in close collaboration with experimentalists.

The annual gross salary of the position amounts to approx 35,000 euros depending on age, experience, and marital status (BAT IIa according to German Salary Scale). The position is immediately available (April 2000). Application from women, minorities and disabled persons are encouraged. The candidates are invited to send their application comprising a curriculum vitae, a list of publications and communications, copies of examination certificates, together with three references, to

Prof. P. Bruno
Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany

The applications can be sent either by conventional mail to the above address or by e-mail as Postscript file(s) to bruno@mpi-halle.de.

POSTDOCTORAL POSITION (COMPUTATIONAL MATERIALS SCIENCE)

THE NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER (NERSC)
LAWRENCE BERKELEY NATIONAL LAB.

http://www.nersc.gov/research/SCG/index.html

The scientific computing group at NERSC has one IMMEDIATE postdoctoral opening in large scale electronic structure calculation and materials simulation. NERSC (http://www.nersc.gov) is the largest civilian research computer center in the United States with a 560 processor T3E machine and a large IBM SP3 machine. The hired person will work with Dr. Andrew Canning and Dr. Lin-Wang Wang in (1) methodology development and implementation of electronic structure calculations (for both ground state and excited states); (2) calculations of real physical problems in collaboration with experimental groups at Lawrence Berkeley lab. The research area we are interested in includes: algorithmic development, large scale calculations, beyond LDA, excited state energy levels, nanostructure, alloys, defects. This position is part of a joint project with Prof. Steven Louie at UC Berkeley, close collaboration with Prof. Louie's group is expected. A Ph.D degree in physics or related field, is required and experience in large scale parallel computation is preferred. The position is initially for one year with the possibility of renewal for up to three years. The salary range is US$4500-$4920/month depending on qualifications. Berkeley is situated in the Bay Area close to San Francisco and Silicon Valley. More information can be found at http://www.lbl.gov/CJO/NE11316.html. Interested persons should send a curriculum vitae (by email) to:

Dr. Andrew Canning
Lawrence Berkeley Lab
1 Cyclotron Road
mail stop 50F
Berkeley, CA 94720
canning@nersc.gov

LBNL is an equal opportunity/affirmative action employer. Clarifications or further details can be obtained via e-mail to canning@nersc.gov or linwang@niche.lbl.gov

Postdoctoral Position

Theoretical Physical Chemistry
Department of Chemistry, University of Pennsylvania

I am looking for a postdoc who will interact productively with an excellent group of Ph. D. students as well as pursue research interests independently. Interested candidates should email their CV, one or two reprints of recent work, and a brief statement of research interests to me at rappe@sas.upenn.edu. Please submit your materials as soon as possible. It will be possible to meet with some candidates at the APS meeting in Minnesota, and candidates not attending the APS meeting will be actively considered as well.

This position has become available because a postdoctoral fellow and a graduate student have recently left my group to start tenure-track faculty position. I am strongly committed to helping each postdoc I work with to achieve his or her career goals. To accomplish this, I involve the postdoc in all aspects of running the group, from setting research goals and supervising students to writing grant proposals. I also invest my time in helping the postdoc to excel in oral presentation of research results for a variety of target audiences, from job talks to national conferences.

My group is involved in three areas of scientific investigation. We study the interactions of molecules with surfaces, using density functional theory and analytical modeling. Our interests in this area include energetic, structural, vibrational, and electronic properties of molecule/surface systems with applications to catalysis, corrosion, epitaxial growth, gas sensing, and tribology. We also investigate the properties of oxide crystals and surfaces with density functional theory. We wish to understand the relationship between the chemical composition of perovskite oxides and their piezoelectric performance, as well how the surfaces of binary oxides catalyze selective oxidation. We have recently begun to examine small gas-phase systems with quantum Monte Carlo methods. We are interested in exploring fundamental van der Waals interactions with these highly accurate quantum-mechanical approaches. In addition to these scientific endeavors, the group is constantly involved in theoretical and computational innovation. For more information, see our group web page: http://lorax.chem.upenn.edu.

Thank you very much for making appropriate candidates aware of this postdoctoral opportunity.

Andrew M. Rappe
Assistant Professor of Chemistry

Positions

Research Training Network EC Contract No:HPRN-CT-1999-00040

Interface analysis at atomic level and Properties of Advanced Materials (IPAM)

Positions are immediately available, eligible young (¡ 35 years) researchers must be citizens of EC or associated countries (Norway, Island, Israel, Lichtenstein, Bulgaria, the Czech Republic, Estonia, Hungary, Lithuania, Poland, Romania, Slovakia, Slovenia and Letonia), however any foreigner who has spent five years in an EC country may apply. Women candidates are particularly encouraged to apply and equal opportunity between women and men will govern our choice. Following the mobility criteria, the young researchers will not apply for a position in their native country.

1. **A full time Ph. D. studentship at Fritz Haber Institute, Max Planck Society, Berlin, Germany**

A three year research studentship position leading to a PhD degree is available at the Fritz-Haber-Institut in Berlin (Germany) in the group "Surface morphology and growth of semiconductors" under the supervision of Dr. Joerg Neugebauer. The research will be mainly focused on the theoretical modeling of electronic properties and atomic structure of interfaces and interfacial defects employing first principles total energy calculations. The basic materials for this project will be gallium nitride based semiconducting layers where extended defects are well known to occur in large concentrations. The research will be performed in close collaboration with experimental, industrial, and theoretical partners within the EC. Strong interaction with the other groups is therefore expected. The succesful candidate will prepare his PhD in environments of Physics, Chemistry and Materials Science, and he/she will earn a strong background on microscopic simulations. Preference will be given to candidates interested in any (or several) of these fields: electronic structure calculations, molecular modeling, density functional theory, empirical potentials, and analysis of transmission electron microscopy measurements.

Interested candidates should send immediately a CV, name and address (including email) of two references, preferably by email or fax, to:

Dr Joerg Neugebauer
E-mail: neugebauer@fhi-berlin.mpg.de,
Phone: ++49 30 8413 4826, Fax: ++49 30 8413 4701,
http://www.fhi-berlin.mpg.de/th/JG

The Candidates will gain time by sending a copy of their CV also to:

Prof. Philomela Komninou,
Leader of the Training Programme,
Tel: +30 31 99 81 95
Fax: +30 31 99 80 61
e-mail: komnhnoy@auth.gr

Please indicate the position of interest.

Tenure-track Assistant Professor

State University of New York-Brockport
Department of Computational Science

http://www.cps.brockport.edu/vacancy.html

Please alert colleagues and graduating students about a faculty vacancy in computational science, posted at SIAM (http://www.siam.org). See below for contact info.

Contact: O. Yasar, Chair, oyasar@brockport.edu .

Research Associate Positions in Ab Initio Simulations

Chair of Theoretical Chemistry at Ruhr-Universitat Bochum (Germany)

Two research associate positions (German nomenclature: prom. wiss. Mitarbeiter, BAT IIa/Ib including full social benefits) are available. The contract will cover one year initially and can be extended up to five years; extension beyond five years is possible via the "Habilitation track". Starting date will be fixed upon mutual agreement. Knowledge of German (written and spoken) is of great advantage, but not strictly required.

Applicants are expected to hold a doctorate in physics or related fields. Expertise in density functional plane-wave pseudo-potential calculations and computational techniques in general is required. Knowledge of molecular dynamics simulations would be helpful.

The interests of the group are covered in a recent review article, "Ab Initio Molecular Dynamics: Theory and Implementation" by D. Marx and J. Hutter in J. Grotendorst (Ed.): "Modern Methods and Algorithms of Quantum Chemistry", p. 301-449, (NIC, Forschungszentrum Julich, 2000), which can be downloaded from
`http://www.fz-juelich.de/wsqc/proceedings/marx.ps`. Further information can be obtained upon email request (unfortunately there is not yet a home page available!).

Interested candidates should send their application (including CV, list of publications with the five most important ones marked, brief outline of research interests and experiences, and two references) before June 2000 preferrentially via snail mail to

Dominik Marx
Lehrstuhl fuer Theoretische Chemie
Ruhr-Universitaet Bochum
44780 Bochum
Germany

Phone : ++49 234 32 28083 (direct)
        ++49 234 32 26485
Fax   : ++49 234 32 14045
Email : dominik.marx@theochem.ruhr-uni-bochum.de

8 Abstracts

Band structure effects in the core level photoemission spectra of NiO

C. A. Rozzi, F. Manghi, C. Arcangeli
Istituto Nazionale per la Fisica della Materia and
Dipartimento di Fisica, Università di Modena e Reggio Emilia,
Via Campi 213/a, I-41100 Modena, Italy

Abstract

Calculation of Ni $2p$ photoelectron spectra for NiO has been performed within a picture which takes into full account the itinerant character of valence electrons and the localised many body interaction between core and valence electrons. The results of an ab-initio band structure calculation are used as an input for the calculation of self-energy correction and spectral function according to a three body scattering solution of a many body Hamiltonian which includes the Coulomb repulsion between core and valence states. The calculated spectrum shows, in agreement with experimental data, a doubly peaked main line which can be attributed to two independent relaxation processes involving valence band Ni d states of either pure or hybridized orbital character.

(Submitted to: Phys. Rev. B - Rapid Commun.)
Latex-file available from: rozzi@unimo.it

Effect of short range order on electronic and magnetic properties of disordered Co based alloys

Subhradip Ghosh, Chhanda Basu Cahudhuri, and Abhijit Mookerjee
S.N. Bose National Centre For Basic Sciences, Calcutta,India
Biplab Sanyal
Department of Physics, Brock University, St. Catharines, Ontario, Canada

Abstract

We here study electronic structure and magnetic properties of CoPd and CoPt alloys using Augmented Space Recursion technique coupled with tight-binding linearized muffin tin orbital (TB-LMTO) method. Effect of short range ordering present in disordered phase on electronic and magnetic properties has been discussed. We show results for Magnetic moment,Curie temperature and electronic band energy with varying degree of short range order at different concentration of Co for both the systems and try to understand and compare the magnetic properties and ordering phenomena in these systems.

(Submitted to Journal of Magnetism and Magnetic Materials)
Latex-file available from : subhra@boson.bose.res.in

Spin–resolved appearance potential spectroscopy investigations on Fe/Cu(001) overlayers

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Butenandtstr. 5-13, D-81377 Munich, Germany
L. Szunyogh*
Center of Computational Materials Science, TU Vienna, Austria
* *Department of Theoretical Physics, TU Budapest, Hungary*
P. Weinberger
Institut für Technische Elektrochemie, TU Vienna, Austria
Center of Computational Materials Science, TU Vienna, Austria
M. Donath
Physikalisches Institut Universität Münster,
Wilhelm–Klemm–Str. 10, D-48149 Münster, Germany

Abstract

The theoretical description of Spin-Resolved Appearance Potential Spectroscopy (SR–APS) developed recently to deal with bulk transition metal systems has been extended to free surfaces of Fe_n/Cu(001). Results of previous experimental work on fcc–Fe on top of a Cu(001)–substrate were interpreted to indicate the coexistence of a few ferromagnetically coupled Fe layers on top of non–ferromagnetic Fe–layers for T=110 K. Recent theoretical work, on the other hand, found for $n > 2$ that the ground–state of this system corresponds to antiferromagnetically coupled Fe layers. In order to clarify this situation the SR–APS spectra of Fe_n/Cu(001) have been calculated assuming the metastable ferromagnetic (FM) as well as antiferromagnetic (AFM) configuration. While for the FM configuration pronounced deviations from experiment were found, a nearly perfect agreement was obtained for the AFM ground–state configuration. This means that the experimental SR–APS spectra are not in conflict with the theoretical prediction but, on the contrary, they strongly support it.

(Submitted to Phys. Rev. B)
Manuscript available as ps-file on request from:
H. Ebert (he@gaia.cup.uni-muenchen.de)

Layer resolved optical conductivity of magnetic multi layers and the *Baukasten principle*

A.Ya. Perlov
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H. Ebert
Institut für Physikalische Chemie, Universität München,
Butenandtstr. 5-13, D-81377 ünchen, Germany

Abstract

The concept of the layer resolved optical conductivity $\boldsymbol{\sigma}^{IJ}(\omega)$ applied by means of a conventional band structure method is introduced. It is demonstrated that it allows for a detailed discussion of the magneto-optical properties of magnetic multi layer systems. In particular it is found that the layer projected optical conductivity $\boldsymbol{\sigma}^{I}(\omega)$ of an atomic layer is influenced by only very few neighboring layers. This property can be exploited within the *Baukasten principle* that aims to predict the magneto-optical properties of a complex layer system from the properties calculated for a closely related but simpler one.

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Spin and orbital magnetic susceptibility of the alloy system $\mathbf{Ag}_x\mathbf{Pt}_{1-x}$

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Dedicated to Prof. J. Voitländer on occasion of his 70th birthday

Abstract

We present results of a first application of linear response formalism to calculate the spin and orbital magnetic susceptibility of a disordered alloy system using the Korringa-Kohn-Rostoker-Coherent Potential Approximation (KKR-CPA). To account for all relativistic effects in a proper way the formalism was used in its fully relativistic version (RKKR-CPA). Results obtained for the alloy system Ag_xPt_{1-x} are presented and compared with experimental data.

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Treatment of non-collinear spin-structures in photo emission and X-ray absorption

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Abstract

Many magnetic compounds possess a non-collinear spin-structure, i.e. the atomic magnetic moments may be oriented with respect to each other in an arbitrary way. When dealing with the electronic structure of such systems this situation can be accounted for in a straightforward way by using the relativistic multiple scattering theory for spin-polarised systems (SPR-KKR). The corresponding formalism is briefly outlined and its application to the studies of the photo emission and X-ray absorption is described. The results of calculations for UPdSn and hcp-Gd are presented.

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Magnetic layers of nickel on copper. Dead or alive?

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Abstract

We studied the perseverance of magnetism in ultrathin nickel films on copper. Layer-dependent magnetic moments in Ni films on the (001), (110) and (111) surface of Cu have been calculated using the Korringa-Kohn-Rostoker Green's function method. The results show that, at temperature $T = 0$, a single nickel monolayer is ferromagnetic on Cu(001) and Cu(110) but magnetically "dead" on more closed-packed Cu(111) surface. Films of two and more layers of Ni are always ferromagnetic with the magnetic moment enhanced in the surface layer but strongly reduced in the interface layer. Due to the short screening length the effect of both the interface and the surface is confined to only a few atomic layers.

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Ab inito thermodynamics and statistics of semiconductor growth, and self-assembly of quantum dots

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Abstract

Recent developments in methodology allow us to extend the *ab initio* (*i.e.*, starting from the self-consistent electronic structure) approach to poly-atomic complexes with 10,000 and more atoms, time-scales of seconds, and involved statistics (*e.g.*, *ab initio* molecular dynamics with 10,000 and more trajectories). In this contribution we will

- sketch recent density-functional theory based hybrid methods, which bridge the length and time scales from those of electron orbitals to meso- and macroscopic proportions,
- present results for crystal growth and the self-assembly of nano-scale structures.

In: Proc. 4th Symposium on Atom-Scale Surface and Interface Dynamics, March 2–3, 2000, Tsukuba, Japan, pp. 3–7.
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Island nucleation in thin-film epitaxy: A first-principles investigation

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Abstract

We describe a theoretical study of the role of adsorbate interactions in island nucleation and growth, using Ag/Pt(111) heteroepitaxy as an example. From density-functional theory, we obtain the substrate-mediated Ag adatom pair interaction and we find that, past the short range, a repulsive ring is formed about the adatoms. The magnitude of the repulsion is comparable to the diffusion barrier. In kinetic Monte Carlo simulations, we find that the repulsive interactions lead to island densities over an order of magnitude larger than those predicted by nucleation theory and thus identify a severe limitation of its applicability.

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Magnetic circular dichroism in Ni $2p$ photoemission of ferromagnetic nickel

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Abstract

The Ni $2p$ photoemission of nickel metal measured with circularly polarized synchrotron radiation is compared with results of spin-polarized relativistic Korringa-Kohn-Rostoker Green's function calculations. The magnetic circular dichroism displays pronounced satellite structures over a wide energy range which are not reproduced by the one-particle calculation. This gives a clear indication for the presence of electron-correlation effects.

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pdf file available from g.vanderlaan@dl.ac.uk or, even better, try electronic journals, J. Phys. Condens. Matter, issue 15, 17th April 2000.

Ab initio theory of perpendicular magnetotransport in metallic multilayers

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Abstract

The current-perpendicular-to-plane (CPP) magnetotransport of a metallic sample sandwiched by two ideal leads is described at an *ab initio* level. The so-called 'active' part of the system is either a trilayer consisting of two magnetic slabs of finite thickness separated by a non-magnetic spacer or a multilayer formed by alternating magnetic and non-magnetic layers. We use a transmission matrix formulation of the conductance based on surface Green functions as formulated by means of the tight-binding linear muffin-tin orbital method. An equivalent and computationally more efficient formulation of the problem based on reflection matrices is also presented. The formalism is extended to the case of lateral supercells with random arrangements of atoms of two types, which in turn allows to deal with ballistic and diffusive transport on equal footing, and which is applicable also to the case of non-collinear alignments of the magnetization in the layers. In addition, for matters of completeness, we present the corresponding expressions for a simple model based on the single-band tight-binding Hamiltonian. Applications refer to fcc-based Co/Cu/Co(001) trilayers and multilayers, considering in detail the effect of substitutional alloying in the spacer and in the magnetic layers, as well as interdiffusion at the interfaces.

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Postscript file is available from: kudrnov@fzu.cz

Valencies in Actinides

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Abstract

The electronic structures of the actinide metals are calculated with the self-interaction corrected local-spin-density approximation. This scheme allows for a splitting of the $5f$ electron manifold into an integral number of localized electrons and a self-consistently determined number of band $5f$ electrons, which hybridize into the non-f derived conduction states. For Pu, Am, Cm, Bk, and Cf, the lowest energy state is obtained when a total of three electrons are available for band formation, while for Es and Fm an additional localized $f-$electron is energetically favorable, leaving only two electrons for band formation. For U and Np, localization is never favored. The present *ab initio* calculations reproduce the trend in valency through the actinide series, and the valency in the actinides is determined by the same rules of hybridization of the f-states as in the rare earths.

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Copy available from: svane@ifa.au.dk

9 Presenting Other Initiatives

Program PHONON for calculating lattice dynamics

An universal program to calculate crystal lattice dynamics of any crystal has been written. The program uses the direct method. To calculate the phonon dispersion relations and/or phonon density of states, it is sufficient to optimize the supercell (which represents a given crystal) by an *ab initio* program, and to calculate the Hellmann-Feynman forces for a small set of supercells, where in each supercell a single atom is slightly displaced from its equilibrium position. During calculations of the Hellamnn-Feynman forces only the optimization of the electronic subsystem must be performed. Then, one should supply to PHONON program the crystal space group, lattice constants, non-equivalent atomic positions, shape of supercell, and the file with the set of Hellmann-Feynman forces. The neighbour list, the symmetry of the force constant matrices and the construction of the dynamical matrix is handled by PHONON. As a result one obtains the phonon dispersion relations and the (partial) phonon density of states, the irreducible representations of all zone center modes, the polarization vectors and atomic displacements for any phonon mode.

The phonon dispersion relations becomes especially useful in the treatment of crystal stability and phase transitions. Thus, the positiveness of all the phonon mode frequencies proves that the system, optimized within constrains of a given space group, is absolutely stable. A negative square phonon mode frequency denotes a soft mode, and suggests an existence of a structural phase transition. Knowing the polarization vectors of the soft mode one may find the space group of a lower symmetry phase. Such calculations are especially useful when studying structural phase transitions as a function of pressure.

The polar crystal usually exhibits the longitudinal/transverse (LO/TO) optical mode splitting, and the direct method cannot handle this splitting. However, PHONON provides a semi-empirical approach to find LO/TO splitting, by supplementing the dynamical matrix with a non-analytical term which depends on the phenomenological effective charges.

PHONON runs on DOS, Windows 95, 98, NT. It has been written by K. Parlinski. If you are interested in PHONON, additional information can be seen at the web page:
http://wolf.ifj.edu.pl/phonon/.

10 SCIENTIFIC HIGHLIGHT OF THE MONTH

FLAPW goes Non-collinear

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Introduction

Non-collinear magnetism in general and incommensurate spin-density waves in particular are complex magnetic structures which exist in a variety of systems. They often occur for topologically frustrated antiferromagnets (e.g. antiferromagnets on a triangular lattice) or materials with competing exchange interactions as for example in the lanthanides. Non-collinear magnetism occurs in spin-glass systems, in domain walls, and is natural for spin fluctuations at finite temperature. The magnetic properties of complex magnets are commonly described within the framework of model Hamiltonians, the simplest of which is the classical Heisenberg model.

In the last years we witnessed a multitude of investigations of non-collinear magnetism in the context of first-principles theory. For instance several *ab initio* calculations have been presented for fcc Fe [1, 2, 3, 4], where solutions of both the spiral spin-density wave and complex non-collinear magnetic structures have been found. Non-collinear magnetic ground states have also been found for more complicated systems such as $MnSn_3$ [5], $ThMn_2$ [6], U_3P_4, U_2Pd_2Sn [7], $YFe_{12-x}Mo_x$ [8], disordered systems [8, 9, 10, 11], multilayers [12, 13] and molecular magnets [14]. Recently, interesting steps have been undertaken to describe the spin-dynamics in itinerant magnets [4, 15]. After the thorough discussion of density functional theory for a non-collinear magnet was completed in [5], these calculations established the density functional theory as a powerful tool to investigate these systems. For a general review see Psi-k Newsletter 14 [16] or the paper by Sandratskii [17].

Common to all of these calculations, which have been carried out using a variety of methods, such as the Korringa-Kohn-Rostoker (KKR) method [1, 18], the Augmented Spherical Wave

(ASW) method [19, 20, 5] or the Linear Muffin Tin Orbital (LMTO) [2, 21] method, is the use of the atomic sphere approximation. That means the space is divided into spheres centered around each atom, wherein there is only one local spin-quantization axis and the corresponding magnetization axis is spherically averaged, $\mathbf{m}(\mathbf{r}) \approx m(r)\hat{\mathbf{e}}_M$. This is consistent with the intuitive picture that each atom carries a magnetic moment and these moments (and their directions) differ between the atoms. Such methods are very suitable to describe the inter-atomic non-collinearity of close-packed systems.

There are, however, problems which call to go beyond the atomic sphere-type of approximation. One of those problems is the investigation of the intra-atomic non-collinear magnetism. This has been pioneered by Nordström *et al.* [22, 23]. Using the full-potential linearized augmented plane wave method (FLAPW), which is free of any shape approximation of the charge- and magnetization density as well as of the potential, the intra-atomic non-collinearity was described taking the full continuous vector spin-density $\mathbf{m}(\mathbf{r})$ into account as it was originally formulated by von Barth and Hedin [24]. It was shown for δ-Pu that due to the interplay of spin-orbit interaction and exchange interaction intra-atomic non-collinearity exists even for ferromagnets.

The frontier field of nanomagnetism creates a second class of interesting problems. In this case we deal with non-collinear magnetism in fairly open structures for which the atomic sphere approximation is known to be less suitable and often provides results with insufficient accuracy. Typical problems are exchange-bias systems [25], technologically important for the magnetic recording industry and the magneto-electronics [26], made out of ferromagnetic films adjacent to antiferromagnetic ones. Recently, we have made an effort to explore this subject using the FLAPW-method, but any other full-potential method capable to deal with magnetism would be equally suitable. In order to deal with non-collinear magnetism of these systems, the Jülich group has extended the film and bulk FLAPW-program `FLEUR` [27] along several directions [28]: (i) to deal with magnetic moments oriented along arbitrary and prescribed directions $\hat{\mathbf{e}}_M^\alpha$ for each atom α, (ii) to deal with the incommensurate spin-spiral state, (iii) and to relax the direction of the magnetic moment self-consistently.

In the following we shortly discuss the implementation of the vector spin-density formalism into the FLAPW-program and go briefly through items (i) and (iii). (ii) the implementation of the spin-spiral states has been nicely discussed in the paper of Andersson *et al.* [29] and is not further mentioned here. At the end we discuss one application, the magnetic spin-structure or an antiferromagnetic monolayer on a triangular lattice: Cr/Ag(111) and Mn/Ag(111).

Implementation of continuous vector spin-density formulation

Non-collinear magnetism has been implemented into two FLAPW codes choosing alternative strategies: Nordström *et al.* [22] work with more physical quantities, the density $n(\mathbf{r})$ and the magnetization density $\mathbf{m}(\mathbf{r})$, and with a spin-independent LAPW basis-set but extended by spin-dependent local orbitals. The implementation of the Jülich group is based on the spin-density matrices and on the standard LAPW basis-set using spin-dependent radial wave functions $u_{\ell\sigma}(r)$ and their energy derivative $\partial u_{\ell\sigma}(r)/\partial E$. The biggest difference, however, arises from the motivation that Jülich group is predominantly interested in the non-collinear magnetism

of $3d$ transition metals at surfaces and in open structures. These are elements with weak intra-atomic non-collinearity. Typically $\mathbf{m}(\mathbf{r})$ is well localized inside the atomic sphere, where $\mathbf{m}(\mathbf{r})$ is essentially parallel to the average of the spin-density of the sphere except in regions close to the sphere boundary where $\mathbf{m}(\mathbf{r})$ is already small. Since in the FLAPW-method the muffin-tin spheres are used which are significantly smaller than volume filling atomic spheres and since the choice of the sphere radii is flexible to a certain degree, but definitely smaller than half the nearest-neighbor distance, we work with a hybrid method: The magnetization is treated as a continuous vector field in the interstitial region and in the vacuum, while inside each muffin-tin sphere we only allow for one direction of magnetization

$$\mathbf{m}(\mathbf{r}) = \begin{cases} \mathbf{m}(\mathbf{r}) & \text{Interstitial and Vacuum} \\ \\ m^{\alpha}(\mathbf{r})\,\hat{\mathbf{e}}_M^{\alpha} & \text{muffin-tin sphere } \alpha \end{cases} . \tag{1}$$

The notation here applies to the FLAPW in the film geometry [30], where the space is partitioned into a film of finite thickness, consisting of an interstitial region and muffin-tin spheres α, and two semi-indefinite vacuum regions on both sides of the film. The continuous vector-field description in the interstitial region describes to a large extent the intra-atomic magnetism of $3d$-metals. This "hybrid" approach is illustrated schematically in Fig. 1.

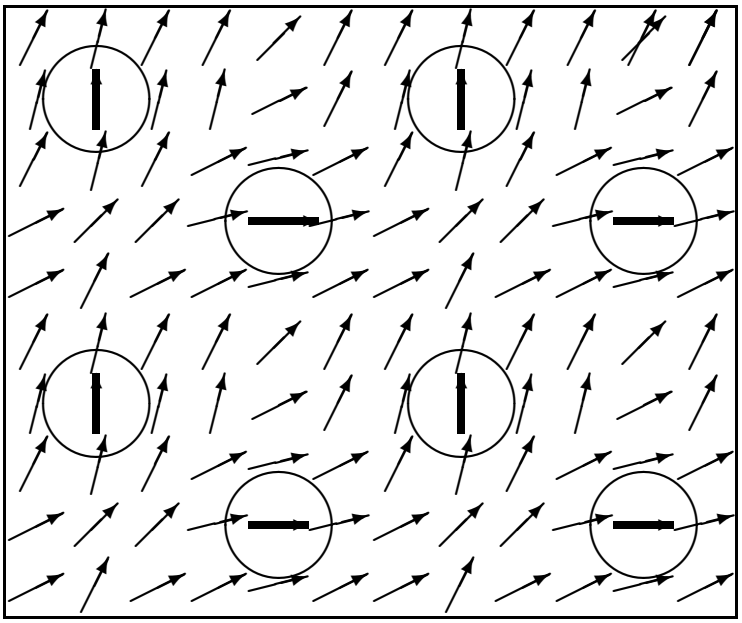

Figure 1: Schematic illustration of the representation of the non-collinear magnetization density within the present approach. The magnetization is treated as a continuous vector field in the interstitial region and in the vacuum. Within each muffin-tin the magnetization has a fixed direction (thick arrows) and can only vary in magnitude. For a better illustration the muffin-tin spheres have been chosen much smaller than in actual calculations.

For chemical elements with a large spin-orbit interaction or off-diagonal intra-atomic Coulomb interaction, one should extend the method to the full vector-field treatment of the magnetization density everywhere in space. To achieve this, it would be necessary to calculate the components of the magnetization that are not parallel to the local quantization axis in the sphere of an atom

and to include the corresponding components of the B-field into the Hamiltonian.

The FLAPW method for collinear calculation uses two sets of radial basis functions inside the muffin-tins for the spin directions. For each spin direction they are set-up using the spherical part of the corresponding potential, $V_\uparrow(r)$ or $V_\downarrow(r)$, and energy parameter, $E_{l\uparrow}$ or $E_{l\downarrow}$. It is still possible to work with $V_\uparrow(r)$ and $V_\downarrow(r)$ in the non-collinear case, since we restrict the magnetization to the local quantization axis. Therefore, a local spin space coordinate frame is introduced with the z-axis parallel to the local quantization axis. $V_\uparrow$ and $V_\downarrow$ are now spin-up and -down with respect to the local axis. Since both, the potential and the basis functions, are set up in terms of the local spin coordinate frame the determination of the basis functions and calculation of the integrals of these functions with the Hamiltonian inside the muffin-tin spheres is completely unchanged. The changes come in, when the basis functions inside the muffin-tins are matched to the plane waves in the interstitial region, because the local spin coordinate frame S^α is rotated with respect to the global frame S^g.

The FLAPW method uses augmented plane waves as basis functions. Therefore, each basis function can be uniquely identified by its wave vector $\mathbf{G}$ and the spin direction. The basis functions in the interstitial region are:

$$e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}\chi_\sigma^g, \tag{2}$$

χ_σ^g is a two component spinor. The index g has been added to notify that χ_σ^g is the representation of this spinor in the global spin frame. This representation is used for both collinear and non-collinear calculations. However in the collinear case, the potential matrix $\mathbf{V}$, and thus the Hamiltonian is block-diagonal in the space spanned by the two spin directions. Therefore, the Hamiltonian can be set-up and solved separately for each of the two spin directions (blocks). In the non-collinear case, $\mathbf{V}$ has off-diagonal parts which are not zero anymore. Hence, the full Hamiltonian for both spin directions are set-up and solved in a single step. In the vacuum region we also use the global spin frame for the representation of the basis functions. Only inside the muffin-tin spheres the basis set is changed, because we use a local spin-coordinate frame, which is rotated with respect to the global frame. The consequence is that, when the functions in the sphere are matched to the plane waves at the boundary of the muffin-tin spheres, each spin direction in the interstitial region is matched to both, the spin-up and -down basis functions, in the sphere. Thus, the basis set has the following form:

$$\varphi_{\mathbf{G},\sigma}(\mathbf{k},\mathbf{r}) = \begin{cases} e^{i(\mathbf{G}+\mathbf{k})\mathbf{r}}\ \chi_\sigma^g & \text{Int.} \\ \left[A_\sigma^{\mathbf{G}}(\mathbf{k}_\parallel)\, u_\sigma^{\mathbf{G}_\parallel}(\mathbf{k}_\parallel,z) + B_\sigma^{\mathbf{G}}(\mathbf{k}_\parallel)\, \dot{u}_\sigma^{\mathbf{G}_\parallel}(\mathbf{k}_\parallel,z)\right] e^{i(\mathbf{G}_\parallel+\mathbf{k}_\parallel)\mathbf{r}_\parallel}\ \chi_\sigma^g & \text{Vac.} \\ \sum\limits_{\sigma^{\mu(\alpha)}}\sum\limits_{L}\left[A^{\alpha\mathbf{G}}_{L\sigma\sigma^{\mu(\alpha)}}(\mathbf{k})\, u^{\alpha(\mu)}_{\ell\sigma^{\mu(\alpha)}}(r) + B^{\alpha\mathbf{G}}_{L\sigma\sigma^{\mu(\alpha)}}(\mathbf{k})\, \dot{u}^{\mu(\alpha)}_{\ell\sigma^{\mu(\alpha)}}(r)\right] Y_L(\hat{\mathbf{r}})\ \chi_{\sigma^{\mu(\alpha)}} & \text{MT}\alpha \end{cases} \tag{3}$$

where $\mathbf{k}$ is the Bloch vector, $\mathbf{G}$ is a reciprocal lattice vector, L abbreviates the quantum numbers l and m, u_l is the regular solution of the radial Schrödinger equation, and $\dot{u}_l$ denotes the energy derivative of u_l. The A- and B-coefficients are determined from the requirement, that the wavefunctions and their derivative have to be continuous at the sphere boundary. The sum in the muffin-tin spheres is over the local spin directions.

After the generalized eigenvalue problem including the full Hamiltonian and overlap matrix

for both spin directions is solved, we obtain the eigenstates of the non-collinear system. The eigenstates are given in terms of the basis functions (3).

$$\psi_\nu(\mathbf{k},\mathbf{r}) = \sum_\sigma \sum_{\mathbf{G}} \mathbf{c}^{\mathbf{G}}_{\nu,\sigma}(\mathbf{k}) \varphi_{\mathbf{G},\sigma}(\mathbf{k},\mathbf{r}). \tag{4}$$

Now the density matrix in the (2×2) spin-space

$$\rho = \frac{1}{2}(n\ I_2 + \boldsymbol{\sigma}\cdot\mathbf{m}) \tag{5}$$

is given by a very simple relation in terms of the solutions of the eigenfunctions

$$\rho_{\alpha\beta} = \sum_{\nu=1}^{N} \psi^*_{\nu,\alpha}\psi_{\nu,\beta}. \tag{6}$$

The potential matrix is defined the same way

$$\mathbf{V} = V\ I_2 + \boldsymbol{\sigma}\cdot\mathbf{B}. \tag{7}$$

Due to the non-collinear magnetism the Hamiltonian has twice the dimension as for the collinear case, the matrix is hermitian, the unit cells become large, the symmetry can become fairly low and often different magnetic states have very similar energies, which requires a large amount of k-points to energetically resolve such magnetic states. Thus the calculations can become rather demanding and the computer codes are parallelized with respect to the number of k-points and eigenstates ν.

Constraint local moments

In general [except for some high symmetry magnetic states e.g. the ferromagnetic state or a particular class of spin-spiral states], an arbitrary magnetic configuration prescribed by a set of magnetization directions $\{\hat{\mathbf{e}}^\alpha_M\}$ are not extrema to the total energy functional $E[n(\mathbf{r}),\mathbf{m}(\mathbf{r})]$. To ensure that the local moments have no components $M^\alpha_\perp$ normal to the directions $\hat{\mathbf{e}}^\alpha_M$, $\hat{\mathbf{e}}^\alpha_\perp$, we work with the constrained DFT [31] in which the total energy for a set of prescribed directions $E(\{\hat{\mathbf{e}}^\alpha_M\})$ is solved, subject to the orientational constraint of the magnetic moments, that $\langle\mathbf{m}^\alpha\rangle\times\hat{\mathbf{e}}^\alpha_M$ is zero for all atoms,

$$E(\{\hat{\mathbf{e}}^\alpha_M\}) = \min\Big\{E[n(\mathbf{r}),\mathbf{m}(\mathbf{r})] + \sum_\alpha \mathbf{B}^\alpha_\perp \langle\mathbf{m}^\alpha\rangle\times\hat{\mathbf{e}}^\alpha_M\Big\}. \tag{8}$$

The Lagrange multipliers $\mathbf{B}^\alpha_\perp$ are transverse constraining fields in the direction $\hat{\mathbf{e}}^\alpha_\perp$. They are obtained self-consistently, simultaneously with the densities. At the end of such a calculation we obtain the self-consistent densities and a set of local constraining B-fields $\{\mathbf{B}^\alpha_\perp\}$ that make the integrated magnetization $\langle\mathbf{m}^\perp_i\rangle$, perpendicular to the local spin quantization axes $\hat{\mathbf{e}}^\alpha_M$, vanish in each muffin-tin sphere.

The effective B-field, $\mathbf{B}^\alpha_{eff}$, that enters the muffin-tin part of the Hamiltonian is given by

$$\mathbf{B}^\alpha_{eff}(\mathbf{r}) = B^\alpha_{xc}\Big(n(\mathbf{r}), m_\parallel(\mathbf{r})\Big)\,\hat{\mathbf{e}}^\alpha_M\ +\ B^\alpha_\perp\,\hat{\mathbf{e}}^\alpha_\perp = B^\alpha_{xc}(\mathbf{r})\,\hat{\mathbf{e}}^\alpha_M\ +\ B^\alpha_\perp\,\hat{\mathbf{e}}^\alpha_\perp = \mathbf{B}^\alpha_{eff}(\mathbf{r})\,\hat{\mathbf{e}}^\alpha_B(\mathbf{r}). \tag{9}$$

In order to calculate the exchange correlation B-field, $\mathbf{B}^\alpha_{xc}(\mathbf{r})$, after the magnetization density is calculated from the wave functions, the magnetization density is projected onto the prescribed local quantization axis $\hat{\mathbf{e}}^\alpha_M$ and we obtain $m^\alpha_\parallel(\mathbf{r})$. Since the exchange correlation B-field is calculated from the projected magnetization density, it is collinear. However, when a constraining field is added, the resulting effective B-field, $\mathbf{B}^\alpha_{eff}(\mathbf{r})$, is again a continuous non-collinear vector field in the muffin-tin spheres, with pointwise local directions $\hat{\mathbf{e}}^\alpha_B(\mathbf{r})$,

$$\hat{\mathbf{e}}^\alpha_B(\mathbf{r}) = \frac{B^\alpha_{xc}(\mathbf{r})\,\hat{\mathbf{e}}^\alpha_M + B^\alpha_\perp\,\hat{\mathbf{e}}^\alpha_\perp}{\left((B^\alpha_{xc}(\mathbf{r}))^2 + (B^\alpha_\perp)^2\right)^{\frac{1}{2}}}, \tag{10}$$

different from the local quantization axis $\hat{\mathbf{e}}^\alpha_M$. Stocks *et al.* [15] noticed this problem and approximated $B^\alpha_\perp$ by an $\mathbf{r}$-dependent functional form $B^\alpha_\perp = c^\alpha\, B^\alpha_{xc}(\mathbf{r})$, where c^α replaces $B^\alpha_\perp$ as the parameter to be determined. This approximation simplifies $\hat{\mathbf{e}}^\alpha_B(\mathbf{r})$ to $\hat{\mathbf{e}}^\alpha_B(\mathbf{r}) \approx \hat{\mathbf{e}}^\alpha_B = (\hat{\mathbf{e}}^\alpha_M + c^\alpha\hat{\mathbf{e}}^\alpha_\perp)/\sqrt{1+(c^\alpha)^2}$, and $\mathbf{B}^\alpha_{eff}(\mathbf{r}) = \sqrt{1+(c^\alpha)^2}\,B_{xc}(\mathbf{r})\,\hat{\mathbf{e}}^\alpha_B$ becomes again collinear within each sphere. The constraining B-fields, $\mathbf{B}^\alpha_\perp$, that enter are often rather small and the approximation suggested by Stocks might be a very good one, although we have not further investigated that. On the other hand due to the introduction of the $\mathbf{r}$-dependence in the constraining fields, the approximation makes the constraining fields inconsistent with the defining equation, Eq. 8. Therefore, we introduce a collinear effective B-field, $\mathbf{B}^\alpha_{eff}(\mathbf{r}) = B^\alpha_{eff}(\mathbf{r})\langle\hat{\mathbf{e}}^\alpha_B\rangle$ in the sphere, by approximating $\hat{\mathbf{e}}^\alpha_B(\mathbf{r})$ by its average direction over the muffin-tin sphere $\langle\hat{\mathbf{e}}^\alpha_B\rangle$, which is independent of $\mathbf{r}$. $\langle\hat{\mathbf{e}}^\alpha_B\rangle = (\hat{\mathbf{e}}^\alpha_M + c^\alpha\hat{\mathbf{e}}^\alpha_\perp)/\sqrt{1+(c^\alpha)^2}$ is defined by replacing the exchange correlation B-field $B_{xc}(r)$ in Eq. 10 by its average over the muffin-tin sphere, $\langle B_{xc}\rangle$, and c^α is now defined as the ratio $c^\alpha = B^\alpha_\perp/\langle B_{xc}\rangle$. For this choice of direction for the effective B-field, the average effective B-field perpendicular to $\langle\hat{\mathbf{e}}^\alpha_B\rangle$, $\langle\hat{\mathbf{e}}^\alpha_B\rangle_\perp$, is zero, $\langle\mathbf{B}^\alpha_{\perp,eff}\rangle = 0$.

Summarizing we can write

$$\mathbf{B}^\alpha_{eff}(\mathbf{r}) = \frac{1}{\sqrt{1+(c^\alpha)^2}}(B^\alpha_{xc}(\mathbf{r}) + c^\alpha B^\alpha_\perp)\langle\hat{\mathbf{e}}^\alpha_B\rangle \qquad \text{with} \qquad \langle\hat{\mathbf{e}}^\alpha_B\rangle = \frac{1}{\sqrt{1+(c^\alpha)^2}}(\hat{\mathbf{e}}^\alpha_M + c^\alpha\hat{\mathbf{e}}^\alpha_\perp). \tag{11}$$

Thus in constrained local moment calculations one works with two slightly different local spin coordinate frames. One of them is given by the direction $\hat{\mathbf{e}}^\alpha_M$ to which the local moment is constrained to, and the other is defined by the average direction $\langle\hat{\mathbf{e}}^\alpha_B\rangle$ of the effective B-field. After the eigenvalue problem has been solved, the solutions are represented within the spin coordinate frame defined by $\langle\hat{\mathbf{e}}^\alpha_B\rangle$, since the Hamiltonian has been setup within that coordinate frame. Hence, when the density matrix is constructed, it is also given with respect to that frame. In order to obtain the density matrix in the spin frame defined by $\hat{\mathbf{e}}^\alpha_M$, it needs to be rotated. To achieve this we first apply the spin-rotation matrix that rotates the density matrix from the coordinate frame $\langle\hat{\mathbf{e}}^\alpha_B\rangle$ to the global spin frame, and then we rotate it again from the global frame to the frame given by $\hat{\mathbf{e}}^\alpha_M$.

Relaxation of the orientation of magnetic moments

In the previous section we have explained how a calculation can be performed where the local magnetic moments are constrained to a set of prescribed directions $\hat{\mathbf{e}}^\alpha_M$. In this section we will show, how the magnetic configuration given by the $\hat{\mathbf{e}}^\alpha_M$ can be relaxed to find a (local) minimum

of the total energy $E\{\hat{\mathbf{e}}_M^\alpha\}$. In such a calculation we also apply the approximation of a collinear magnetization density inside each muffin-tin sphere, $\mathbf{m}(\mathbf{r}) = m^\alpha(\mathbf{r})\hat{\mathbf{e}}_M^\alpha$, only the directions $\hat{\mathbf{e}}_M^\alpha$ (and consequently $m^\alpha(\mathbf{r})$) are relaxed. In order to relax the magnetic configuration it is necessary to calculate the total (integrated) perpendicular output magnetization:

$$\langle \mathbf{m}_{\perp,out}^\alpha \rangle = \int_{MT_\alpha} \mathbf{m}_{\perp,out}^\alpha(\mathbf{r})\, d^3r. \tag{12}$$

This quantity is easier to calculate than the perpendicular magnetization density $\mathbf{m}_{\perp,out}^\alpha(\mathbf{r})$, since only the spherical part, $\mathbf{m}_{\perp,out}^\alpha(r)$, of the perpendicular magnetization density is needed to calculate the integrated quantity. The integrated parallel magnetic moment is calculated just as in a collinear calculation,

$$\langle \mathbf{m}_{\parallel,out}^\alpha \rangle = M^\alpha \hat{\mathbf{e}}_M^\alpha = \int_{MT_\alpha} \mathbf{m}_{\parallel,out}^\alpha(\mathbf{r})\, d^3r = \int_{MT_\alpha} m_{\parallel,out}^\alpha(\mathbf{r})\, \hat{\mathbf{e}}_M^\alpha\, d^3r. \tag{13}$$

The output direction $\hat{\mathbf{e}}_{out}^{\alpha,(i)} = (\langle \mathbf{m}_{\perp,out}^\alpha \rangle + \langle \mathbf{m}_{\parallel,out}^\alpha \rangle)/|\langle \mathbf{m}_{\perp,out}^\alpha \rangle + \langle \mathbf{m}_{\parallel,out}^\alpha \rangle|$ at each site α differs normally from the input direction (the orientation of the spins at the beginning of the iteration step i), $\hat{\mathbf{e}}_{in}^{\alpha,(i)}$. For the next iteration $i+1$, the input direction $\hat{\mathbf{e}}_{in}^{\alpha,(i+1)}$ is changed independently of the charge density and the size of the magnetizations, $|\langle \mathbf{m}_{\perp,out}^\alpha \rangle|$ or $|\langle \mathbf{m}_{\parallel,out}^\alpha \rangle|$. In our implementation the parameters describing the orientation are the azimuthal and polar angles φ and θ, respectively. As a first and successful approach we used straight mixing to determine the input orientation for the next iteration step: For example the angle $\varphi_{in}^{\alpha,(i+1)}$ being used in the next iteration is chosen as:

$$\varphi_{in}^{\alpha,(i+1)} = (1-\beta)\, \varphi_{in}^{\alpha,(i)} \; + \; \beta\, \varphi_{out}^{\alpha,(i)}, \tag{14}$$

where β is a mixing parameter, which is chosen to obtain fast convergence. Convergence of the charge and magnetization density, and the directions can be done simultaneously, i.e. after each self-consistency iteration of the densities a new set of angles is determined. The mixing scheme as well as the mixing parameters are chosen independently for the densities and the directions. However, when a Broyden mixing scheme is used for the densities, the Broyden "memory" has to be deleted regularly (every 10 iterations) while the directions are still changing quickly.

As a test system for this implementation we have chosen fcc-Co (cf. Fig. 2), because it is well known that fcc-Co has a ferromagnetic ground state. The self-consistent determination of the relative ground-state angles between these two atoms was started using a converged charge density for the particular relative angle of $\frac{\pi}{2}$ between the orientation of the magnetic moments. Then the variation of the orientation is carried out as described above. We used $\beta = 3.0$, which means that the mixing is even more than 100% for the directions of the local moments. The change of the angle between both spins is shown in Fig. 3. From Fig. 3 it can be seen clearly, that the convergence of the orientation is very fast. In the above example the expected ferromagnetic state is reached after only 5 iterations. Due to the fast change of the directions, the charge $n(\mathbf{r})$ and magnetization density $m_{(\parallel)}(\mathbf{r})$ are not converged anymore and further 15 iterations are needed basically to converge those quantities. After 20 iterations both, the densities and the directions are converged. This shows that by separating the orientational degrees of freedom of the magnetic moment from the charge-density and the size of the magnetization during the iteration-progress, the convergence of the orientation of spins can be considerably accelerated.

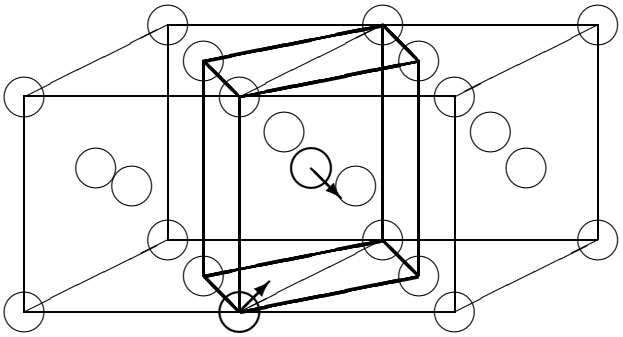

Figure 2: Fcc-lattice with the bct-unit cell (bold lines) containing two atoms. The arrows indicate the direction of the magnetic moments at each site in this unit-cell.

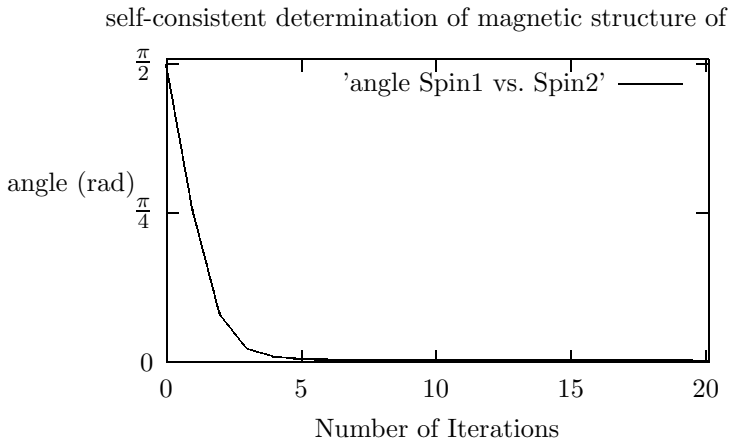

Figure 3: The calculations were performed for fcc-Co with the experimental lattice-constant of $a_0 = 6.70$ a.u. using a bct unit-cell, containing two Co-atoms. The graph shows the evolution of the relative angle between both magnetic moments (see Fig. 2.) plotted as a function of the number of iterations.

Application: Monolayers of Cr and Mn at Ag(111)

Background

In the past ultra-thin $3d$ transition-metal films, grown on oriented single-crystal noble-metal substrates, attracted much attention as they exhibit itinerant magnetism and are thus physical realizations of two-dimensional magnetic models. Most experimental and theoretical work focused on overlayers on (001) substrates. The theoretical studies [33] have predicted greatly enhanced magnetic moments in the overlayer and even more importantly two competing magnetic phases in the monolayer: the c(2×2) antiferromagnetic structure for V, Cr, and Mn monolayers and the p(1×1) ferromagnetic structure for Fe, Co, and Ni monolayers. As a result of this investigation we can conclude that the magnetic in-plane nearest-neighbor (n.n.) exchange interaction of V, Cr, and Mn is antiferromagnetic.

Antiferromagnetic interactions on a triangular lattice are the origin of frustrated spin systems. A triangular lattice is provided for example by (111) oriented fcc substrates, e.g. Ir(111) [34] or noble metals or by (0001) oriented hcp substrates, e.g. Ru(0001) [35]. The classical n.n. Heisenberg model predicts a two-dimensional non-collinear ground state for the triangular lattice, commonly called the Néel state. This configuration has three atoms in a $(\sqrt{3} \times \sqrt{3})$R30° unit cell with the magnetic moments of the three atoms aligned at $\pm 120°$ with respect to the neighboring atoms.

In fact, triangular antiferromagnets can be crystallized e.g. in the form of stacked antiferromagnets. A typical compound is $LiCrO_2$ [36] and this is a compound with *localized* spins. It seems that in many cases the magnetic interaction of localized spins are well described by the (n.n.) Heisenberg model. The systems we are investigating are *itinerant* antiferromagnets on a triangular lattice and it is by no means clear how far a short-ranged n.n. interaction or even how far the Heisenberg model can go in giving a sufficiently good description of the physics of itinerant magnets on a triangular lattice.

Therefore we investigated the ground-state spin structure of Cr and Mn monolayers beyond the Heisenberg model by performing *ab initio* calculations based on the density functional theory. We concentrate here on the discussion of unsupported (free standing) (111) monolayers (UML) of Cr and Mn with the lattice constant of Ag(111). Repeating the investigations with and without an Ag substrate does not alter the results qualitatively.

Results

The following different magnetic structures are compared: (i) The ferromagnetic p(1×1) structure. (ii) The row-wise antiferromagnetic structure as shown in Fig. 4a. The unit cell of this configuration contains 2 atoms (cf. Fig. 4c). The ferromagnetic structure and the antiferromagnetic structure is connected by a continuous rotation as indicated in Fig. 4c. (iii) The 120° configuration or the Néel state, respectively, which the n.n. Heisenberg model predicts to be energetically preferable for antiferromagnetic materials. The corresponding $(\sqrt{3} \times \sqrt{3})$R30° unit cell is shown in Fig. 4d. It is again possible to go from the ferromagnetic structure to the 120° configuration by a continuous rotation, rotating two atoms by the same angle φ but in opposite

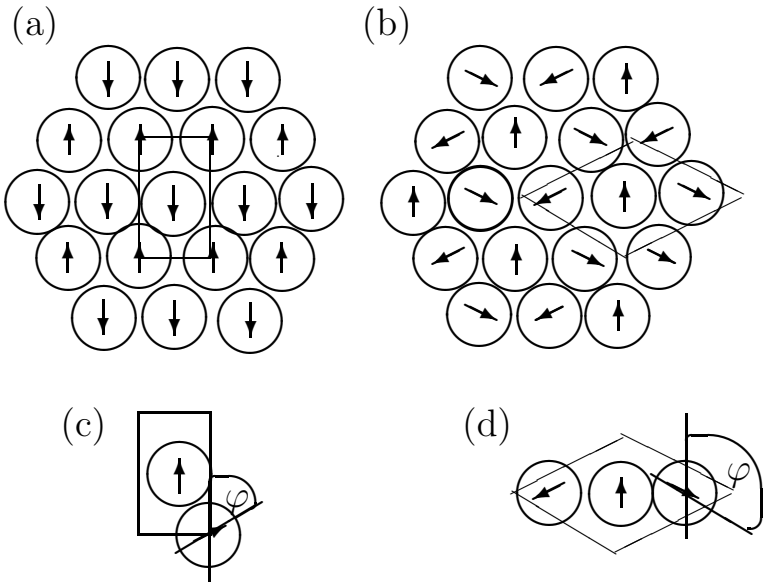

Figure 4: Magnetic structures of hexagonal monolayers: a) The row-wise antiferromagnetic structure. b) The non-collinear 120° configuration. The ferromagnetic structure can be transformed by a continuous rotation into structure a) as indicated in c) and into structure b) as indicated in d).

directions, as indicated in Fig. 4d. If this rotation is continued up to $\varphi = 180°$, the system arrives at an additional collinear antiferromagnetic structure, or more accurately an antiferr**i**magnetic structure, which will be denoted as the 180° configuration. A $k_\parallel$-point set that corresponds to 180 $k_\parallel$-points in the full two-dimensional Brillouin zone has been used for the unit cell containing two atoms, while the $k_\parallel$-point set for the $(\sqrt{3} \times \sqrt{3})$R30° unit cell corresponds to 121 $k_\parallel$-points in the full Brillouin zone. It has been checked very carefully that the total energy differences calculated in the two different unit cells are comparable (in particular with respect to the $k_\parallel$-point convergence), by comparing the energy difference between the non-magnetic and ferromagnetic configuration in both unit cells.

The results of the calculations are presented in Fig. 5. The plots show the total energy as a function of the rotation angle φ. The left panels show rotations that transform the ferromagnetic structure into the row-wise antiferromagnetic structure. The right panels show the rotations according to Fig. 4d. The scales of the left and right panels are equal, they differ, however, between Cr (upper panels) and Mn (lower panels).

Consider first Cr: Starting from the row-wise antiferromagnetic solution (Fig. 5 upper left panel), and rotating towards the ferromagnetic structure, the energy shows a cosine-like behavior, as the n.n. Heisenberg model predicts for an antiferromagnet. The total energy along the rotation path in the unit cell of Fig. 4d (Fig. 5 upper right panel) reveals a pronounced minimum at 120°. This minimum and shape of the energy curve matches nicely the expectation from the Heisenberg model. It is clearly visible that the 120° configuration is the lowest energy configuration among all configurations studied here. Thus, the magnetic Néel state is the ground state of the Cr UML predicted by the present investigation.

Now turning to Mn and comparing the results in the two-atom unit-cell (Fig. 5 lower left panel)

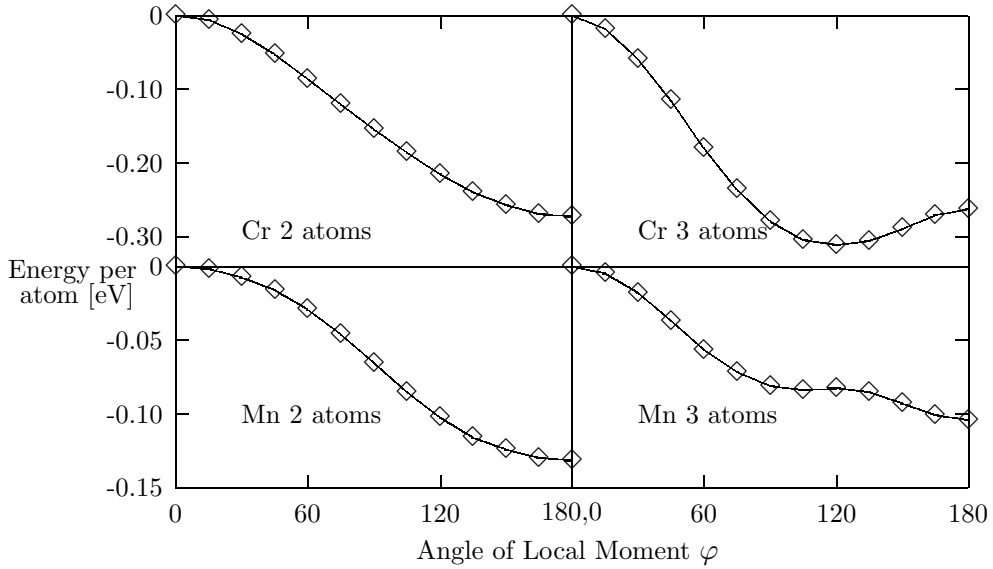

Figure 5: Calculated energy as function of the rotation angle of the local moment for the UML of Cr (upper panels) and Mn (lower panels) with the Ag(111) geometry.

with those of Cr (Fig. 5 upper left panel) we find that the behavior of Mn and Cr is very similar, i.e. the energy curve is cosine-like and Mn prefers to be antiferromagnetic. The calculations reveal, however, two surprises: (i) The lowest energy configuration among all magnetic structures investigated is the row-wise antiferromagnetic configuration. (ii) The total energy of the Mn system with 3 atoms per unit cell does not exhibit a minimum at 120°, as should be expected from the n.n. Heisenberg model, but a local maximum. Apparently, the 180° configuration is lower in energy than the Néel state (120° configuration). In summary, the lowest energy configuration, among all magnetic structures investigated, is the row-wise antiferromagnetic configuration.

From these results we can draw two conclusions:
(i) Since the row-wise antiferromagnetic configuration is lower in energy than the Néel state, the exchange interaction beyond nearest neighbors is important. Thus we cannot *a priori* exclude the possibility of even more complicated spin structures that have been ignored so far. The most probable ones are the incommensurate spin-spiral states along the high-symmetry lines in the two-dimensional Brillouin zone for the spin-spiral wave vectors. We have investigated the total energy along those high-symmetry lines and found that the row-wise antiferromagnetic state (high-symmetry point in the two-dimensional Brillouin zone) has the lowest energy among all spin-spiral wave vectors on high-symmetry lines.
(ii) Within the Heisenberg model the energy $E(\varphi)$ is either proportional to $\cos(\pm\varphi)$ or $\cos(\pm 2\varphi)$. A functional form consisting of these terms cannot fit the local maximum at 120° for Mn. Motivated by the perturbative treatment of the Hubbard-model [37] in case of strong Coulomb-interaction in which the Heisenberg Hamiltonian is derived in second order perturbation, and the lowest order correction to the Heisenberg model is due to four-spin interactions, we suggested in Ref. [38] that the maximum at 120° is due the four-spin interactions. The classical Hamiltonian

describing the four-spin interaction reads

$$H_{4\text{-}spin} = -\sum_{ijkl} K_{ijkl}[(\mathbf{S}_i\mathbf{S}_j)(\mathbf{S}_k\mathbf{S}_l) + (\mathbf{S}_j\mathbf{S}_k)(\mathbf{S}_l\mathbf{S}_i) - (\mathbf{S}_i\mathbf{S}_k)(\mathbf{S}_j\mathbf{S}_l)]. \quad (15)$$

Within the n.n. approximation ($K_{ijkl} = K_1$), the energy of the four-spin interaction in the three-atom unit-cell exhibit exactly a functional form $E(\varphi) \propto \cos 3\varphi$.

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