Ψ_k Newsletter

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

Number 70 August 2005

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Contents

1 Editorial

In this newsletter we have two workshop/conference reports, including abstracts of presented papers. These are followed by a number of conference and position announcements. Abstracts of recent or newly submitted papers are preceding the scientific highlight which is on "Diluted Magnetic Semiconductors" by K. Sato, H. Katayama-Yoshida (Osaka) and P.H. Dederichs (Juelich). Please check the table of contents for further details.

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

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

The above contains information on the Psi-k 2005 workshops and hands-on courses (subject to funding). In these pages you can also find information on how to apply for funding to make collaborative visits.

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

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

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

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

2 News from the ESF Programme

"Towards Atomistic Materials Design"

2.1 Reports on ESF Psi-k Workshops/Conferences

2.1.1 Report on the European Conference: PHYSICS OF MAGNETISM'05

24-27 June, 2005 Poznań, Poland

Co-sponsored by the European Science Foundation Psi-k Programme

Towards Atomistic Materials Design

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

The European Conference Physics of Magnetism'05 was held in Poznań from 24-th to 27-th June 2005. The Conference was the eleventh of the series organised every three years since 1975 jointly by the Institute of Molecular Physics Polish Academy of Sciences and the Institute of Physics Adam Mickiewicz University.

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

-novel metallic oxides and magnetoresistive materials

-high temperature superconductors

-low dimensional quantum magnets

-heavy fermions, fluctuating valence and Kondo systems

-spintronics, nanomagnetism and nanostructures

-magnetic semiconductors

-surfaces and multilayers

-electronic structure

The main objective of the Conference was to bring together scientists and technologists from the Western, Central and Eastern European countries involved in research and applications of new magnetic materials and high temperature superconductors. 222 researchers from 17 countries spent four days discussing physics of new magnetic materials.

The plenary talks were presented by 28 invited scientists: 12 from Germany, 6 from Poland, 2 from USA, Japan and France, and 1 from Slovakia, Switzerland, Italy and England.

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

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

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

http://www.ifmpan.poznan.pl/zp2/pm05.html

Andrzej Jezierski (Poznań)

SCHEDULE

Friday, June 24

8^{50}-9^{00} OPENING

R. Micnas, A. Jezierski

I.1 STRONGLY CORRELATED ELECTRONS

Chairmen: R. Micnas, A. Jezierski

9^{00}-9^{30} **W. METZNER** *(invited speaker)*

Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Magnetic and superconducting correlations in the 2D Hubbard model

9^{30}-10^{00} **B.R. Bułka** *(invited speaker)*

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

Correlations in electronic transport through nanostructures

10^{00}-10^{30} **P. HORSCH** *(invited speaker)*

Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Magnetism and charge response in quasi-1d Wigner lattice compounds

10^{30}-11^{00} **B. DĄBROWSKI** *(invited speaker)*

Physics Department, Northern Illinois University, DeKalb, USA

Magnetic properties of nonstoichiometric and substituted $SrRuO_3$

11^{05}-11^{30}coffee break

I.2 MOSTLY MAGNETIC NANOSTRUCTURES

Chairman: H. Szymczak

11^{30}-12^{00} **G. BAYREUTHER** *(invited speaker)*

Institut für Experimentelle und Angewandte Physik,

Universität Regensburg, Regensburg, Germany

Ground state properties and spin excitations in ferromagnetic nanostructures

12^{00}-12^{30} **A. EHRESMANN** *(invited speaker)*

Fachbereich Naturwissenschaften, Universität Kassel, Kassel, Germany

In-plane magnetic micro- and nanopatterns: fundamentals, applications, and possibilities

12^{30}-13^{00} **A. MAZIEWSKI** *(invited speaker)*

Institute of Experimental Physics, University of Białystok, Białystok, Poland

New spin configurations in nano-sized magnets near reorientation phase transitions

13^{00}-13^{30} **M. MIGLIERINI** *(invited speaker)*

Department of Nuclear Physics and Technology,

Slovak University of Technology, Bratislava, Slovakia

Magnetic microstructure of NANOPERM-type nanocrystalline alloys

13^{35}-15^{00} lunch break

15^{00}-16^{40} **ORAL SESSIONS** (concurrent)

O1 Chairman: K.I. Wysokiński (Auditorium Maximum)

O-1-15 J. Stankowski:

Fluctuation of Cooper pairs

O-1-07 A. M. Oleś, L.F. Feiner, P. Horsch, and G. Khaliullin:

Microscopic theory of magnetic interactions in $KCuF_3$ and $LaMnO_3$-the role of charge transfer

O-1-03 I. Eremin, D. K. Morr, A. V. Chubukov, D. Manske,

K. H. Bennemann, M. R. Norman:

Resonant magnetic excitations in high-T_c cuprates: influence of orthorhombicity and upward dispersion

O-1-09 T. Domański:

Quantum fluctuations of the ultracold atom-molecule mixtures

O-1-12 L. Kowalewski, R. J. Wojciechowski and P. Wojtuś:

Andreev reflection at ferromagnetic metal- triplet superconductor junctions

O-1-14 P. Wróbel, A. Maciąg and R. Eder:

Single particle spectral weight and ARPES spectra from cuprates in the bond-ordered, bond-centered stripe phase

O2 Chairman: A. Ślebarski (Lecture room A)

O-4-05 B. Andrzejewski, A. Kowalczyk, J. Frąckowiak, A. Szlaferek, S. Pal, Ch. Simon:

Unusual negative magnetisation effect in antiferromagnetic $YbFe_4Al_8$ compound

O-2-04 H. Wende, A. Scherz, C. Sorg, P. Jensen, M. Bernien, N. Ponpandian, K. Baberschke:

Importance of spin fluctuations in coupled two-dimensional magnetic trilayers

O-2-08 S. van Dijken, M. Żołądź, M. Czapkiewicz, T.Stobiecki:

Asymmetric magnetization reversal in exchange-biased Co/Pt multilayers

O-2-09 M. Czapkiewicz, S. van Dijken, T. Stobiecki, R. Rak, M. Żołądź and P. Mietniowski:

Magnetization dynamics of perpendicular exchange -biased (Pt/Co)-Pt-IrMn multilayers studied by MOKE microscopy and magnetometry

O-3-01 G. Pristáš, M. Reiffers, J. Šebek, E. Šantavá, K. Andersen and B. Hamelin:

Electron-quasiparticle interaction in van Heusler alloy Cu_2MnAl

16^{40}-17^{00} coffee break

17^{00}-18^{30} **POSTER SESSION I** (categories 2, 6, 7)

18^{45}-20^{15} **WELCOME PARTY**

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Saturday, June 25

I.3 HIGH TEMPERATURE SUPERCONDUCTORS

Chairman: S. Robaszkiewicz

9^{00}- 9^{30} **K. MAKI** *(invited speaker)*

Department of Physics and Astronomy, University of Southern California, Los Angeles, USA

D-wave density waves in high T_c cuprates and $CeCoIn_5$

9^{30}-10^{00} **C. DI CASTRO** *(invited speaker)*

Dipartimento di Fisica, Universita' di Roma "La Sapienza", and Istituto Nazionale per la Fisica della Materia, Rome, Italy

Charge-ordering fluctuations and anomalous Raman response in cuprates

10^{00}-10^{30} **S. MAEKAWA** *(invited speaker)*

Institute for Materials Research, Tohoku University, Sendai, Japan

Spin-charge separation and non-linear optical response in one-dimensional cuprates

10^{30}-11^{00} **D. POILBLANC** *(invited speaker)*

Laboratoire de Physique Théorique, Université Paul Sabatier and CNRS, Toulouse, France

Doped 2D frustrated quantum magnets: spin-charge separation and non-conventional superconductivity

11^{05}-11^{30}coffee break

I.4 MOSTLY MAGNETIC PROPERTIES

Chairman: J. Baszyński

11^{30}-12^{00} **K. DÖRR** *(invited speaker)*

Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden,

Dresden, Germany

Magnetism in manganites and manganite-titanate biferroics

12^{00}-12^{30} **S. BLÜGEL** *(invited speaker)*

Institut für Festkörperforschung, Forschungszentrum Jülich,

Jülich, Germany

Magnetic tunneljunctions made from half-metals

12^{30}-13^{00} **H. EBERT** *(invited speaker)*

Department Chemistry/Physical Chemistry,

Ludwig-Maximilians-University of Munich, Munich, Germany

Relativistic and correlation effects in magnetic solids

13^{00}-13^{30} **R. WIESENDANGER** *(invited speaker)*

Institute of Applied Physics and Microstructure Advanced Research Center

Hamburg (MARCH), University of Hamburg, Hamburg, Germany

Physics of nanomagnetism revealed by spin-polarized scanning tunneling spectroscopy

13^{35}-15^{00} lunch break

15^{00}-16^{25} **ORAL SESSIONS** (concurrent)

O3 Chairman: B. Fechner (Auditorium Maximum)

O-2-05 P. Stefański, A. Tagliacozzo and B.R. Bułka:

"Charge sensing" effects in conductance through quantum dots and point contacts

O-2-10 K.-I. Imura and R. Shindou:

Wave-packet dynamics of Bloch electrons - role of Berry phase

O-2-11 T. Story, P. Dziawa, V. Osinniy, M. Arciszewska,

W. Dobrowolski, W. Domuchowski, K. Dybko,

O. Fedorych, E. Łusakowska, B. Taliashvili, C.J.P. Smits,

H.J.M. Swagten:

Ferromagnetic (Eu,Gd)Te semiconductor layers

O-2-12 J. Martinek, J. Barnaś, J. König, G. Schön, S. Maekawa,
J. von Delft, D.C. Ralph:

Kondo effect in the presence of ferromagnetism mixtures

O-2-15 J.-C. S. Levy and A. Ghazali:

Monte- Carlo simulation of solid state and melting of 2D confined magnetic particles

O4 Chairman: L. Wojtczak (Lecture room A)

O-1-01 A. Szewczyk, M. Gutowska, and B. Dąbrowski:

Phase diagram of heavily doped ($x > 0.5$) $La_{1-x}Sr_xMnO_3$

O-1-05 A. Wiśniewski, R. Puźniak, V. Markovich, I. Fita,
Ya.M. Mukovskii:

Pressure effects on magnetic properties of manganites near percolation threshold

O-1-06 R. Puźniak, A. Wiśniewski, J. Jun, S.M. Kazakov,
J. Karpiński:

Influence of chemical substitutions on anisotropic upper critical field in MgB_2: impact of Fermi surface changes

O-1-08 V. H. Tran, S. Paschen, F. Steglich, R. Troć,
and Z. Bukowski:

Hall effect in the low charge-carrier density ferromagnet $UCo_{0.5}Sb_2$

O-1-11 V.Yu. Ivanov, A.A. Mukhin, V.D. Travkin, A.S. Prokhorov,
A.M. Kadomtseva, Yu.F. Popov, G.P. Vorobev,
K.I. Kamilov, and A.M. Balbashov:

New orthorhombic multiferroics $R_{1-x}Y_xMnO_3$ (R = Eu; Gd)

16^{30}-17^{15} **TRANSPORTATION TO PALACE IN KÓRNIK**

18^{00}-21^{00} **BANQUET**

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Sunday, June 26

I.5 MOSTLY DILUTED MAGNETIC SEMICONDUCTORS, SPINTRONICS AND MIXED VALENCE

Chairman: S. Krompiewski

9^{00}- 9^{30} **T. DIETL** *(invited speaker)*

Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Carrier-controlled ferromagnetic semiconductors

9^{30}-10^{00} **B.L. GALLAGHER** *(invited speaker)*

School of Physics & Astronomy, University of Nottingham, Nottingham, UK

GaMnAs materials and nanoscale devices

10^{00}-10^{30} **P. DEDERICHS** *(invited speaker)*

Institut für Festkörperforschung, Forschungszentrum Jülich,

Jülich, Germany

Percolation effects in dilute magnetic semiconductors

10^{30}-11^{00} **P. WACHTER** *(invited speaker)*

Laboratorium für Festkörperphysik, ETH Zürich, Zürich, Switzerland

Superfluidity in condensed excitons below 20 K

11^{05}-11^{30}coffee break

11^{30}-13^{40} **ORAL SESSIONS** (concurrent)

O5 Chairman: A.M. Oleś (Auditorium Maximum)

O-1-13 C. Knecht, N. Blümer, and P.G.J. van Dongen:

Orbital-selective Mott transitions in the anisotropic two-band Hubbard model at finite temperatures

O-7-02 R. Eder and H. Winter:

Cluster perturbation theory for transition metal oxides

O-7-01 P. Kratzer, H. Wu, J. Hashemifar, M. Hortamani and M. Scheffler:

Calculation of structural, electronic and magnetic properties of MnSi and Co_2MnSi(001) thin films

O-2-14 A. Rycerz and J. Spałek:

Electronic structure and parity effects in correlated nanosystems

O-6-02 R. Lemański and P. Mikołajczyk:

Magnetic properties of correlated electrons

O-2-13 S. Krompiewski, G. Cuniberti, and N. Nemec:

Spin transport in disordered single-wall carbon nanotubes contacted to ferromagnetic leads

O-3-02 G.A. Gehring, A. Lehmann-Szweykowska, R.J. Wojciechowski, P.E.Wigen and R. Micnas:

Charge transport through ionic clusters of the magnetic oxides

O6 Chairman: Z. Jacyna-Onyszkiewicz (Lecture room A)

O-6-01 M.W. Gutowski:

On the symmetry of a Preisach map

O-3-03 I. Škorvánek, J. Marcin, T. Krenický, J. Kováč, P. Švec and D. Janičkovič :

Improved soft magnetic properties in hitperm nanocrystalline alloys by heat treatment under external magnetic field

O-3-06 J. Przewoźnik, Cz. Kapusta, J. Żukrowski, K. Krop, M. Sikora, D. Rybicki, D. Zając, B. Sobanek, C.J. Oates, P.C. Riedi:

On the strength of the double exchange and superexchange interactions in $La_{0.67}Ca_{0.33}Mn_{1-y}Fe_yO_3$ - an NMR and Mössbauer study

O-1-10 R. Zalecki, A. Kołodziejczyk, J. Korecki, A. Kozłowski, N. Spiridis and Z. Kąkol:

Electronic states of magnetite from electron photoemission spectroscopy

O-2-01 V.K. Dugaev, P. Bruno, M. Taillefumier, B. Canals, and C. Lacroix:
Intrinsic mechanism of anomalous Hall effect in a two-dimensional magnetic system with impurities

O-4-01 B. Idzikowski, A. Kreyssig, M. Loewenhaupt, Z. Śniadecki, A. Hoser, K.-H. Müller:
Magnetic structures in cubic RCu_5 (R=Tb, Dy, Ho) compounds

O-4-02 A. Szytuła, D. Kaczorowski and B. Penc:
Electronic structure of RAg_2Ge_2 (R = Pr, Nd) compounds

13^{40}-15^{00} lunch break

15^{00}-16^{30} **POSTER SESSION II** (categories 1, 3, 4, 5)

Free time

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Monday, June 27

I.6 SPIN DEPENDENT TRANSPORT, MAGNETIC JUNCTIONS AND MAGNETIC LAYERS

Chairman: J. Barnaś

9^{00}- 9^{30} **A. FERT** *(invited speaker)*
Unité Mixte de Physique CNRS-Thomson CSF, Orsay, France
Magnetization reversal by injection and transfer of spin: experiments and theory

9^{30}-10^{10} **S. YUASA** *(invited speaker)*
National Institute of Advanced Industrial Science and Technology (AIST) Tsukuba, Japan and PRESTO, Japan Science and Technology Agency (JST), Saitama, Japan
Giant room-temperature TMR effect in magnetic tunnel junctions

with MgO(001) tunnel barrier

10^{00}-10^{30} **B. HILLEBRANDS** *(invited speaker)*

Fachbereich Physik, Technische Universität Kaiserslautern,

Kaiserslautern, Germany

Propagation, tunneling and phase shift of spin waves at a magnetic field inhomogeneity

10^{30}-11^{00} **H. PUSZKARSKI** *(invited speaker)*

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

Magnetic excitations in magnonic crystals and in small magnetic particles

11^{05}-11^{30} coffee break

I.7 LOW DIMENSIONAL MAGNETISM

Chairman: L. Kowalewski

11^{30}- 12^{00} **R.K. KREMER** *(invited speaker)*

Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Frustrated antiferromagnetic quantum chain systems

12^{00}-12^{30} **J. SZNAJD** *(invited speaker)*

W. Trzebiatowski Institute for Low Temperature and Structure Research,

Polish Academy of Sciences, Wrocław, Poland

Renormalization group approach to weakly interacting spin and Fermion chains

12^{30}-13^{30} **ORAL SESSION**

O-4-04 R. Troć, Z. Bukowski, C. Sułkowski, J.Stępień-Damm:

Magnetic and transport properties of Cu-flux-grown UCu_2Si_2

O-1-02 A. Ślebarski and K. Szot:

Non-Fermi liquid ground state in CeRhSn: effect of grain boundary defects on the electric transport behavior

O-1-04 T. Cichorek, A.C. Mota, F. Steglich,

N.A. Frederick, W.M. Yuhasz and M.B. Maple:

Low-field magnetic investigations of the superconducting state in $PrOs_4Sb_{12}$

13^{30}-15^{00} lunch break

I.8 MOSTLY HEAVY FERMION SYSTEMS

Chairman: R. Troć

15^{00}-15^{30} **F. STEGLICH** *(invited speaker)*

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

Unconventional forms of superconductivity and quantum criticality in heavy-electron metals

15^{30}-16^{00} **J. SPAŁEK** *(invited speaker)*

M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland

Magnetic properties of almost localized Fermions - revisited

16^{00}-16^{20} SUMMARY (J. SPAŁEK-theory, J. DUBOWIK-experiment)

16^{20}-16^{30} CLOSING (R. Micnas, A. Jezierski)

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PM'05 – INVITED LECTURES

(abstracts)

GROUND STATE PROPERTIES AND SPIN EXCITATIONS IN FERROMAGNETIC NANOSTRUCTURES

G. Bayreuther

Institut für Experimentelle und Angewandte Physik
Universität Regensburg
D-93040 Regensburg, Germany

The confinement of electrons in one or more dimensions of space in ferromagnetic nanostructures has pronounced consequences for most magnetic properties. The reason is the cooperative or collective nature of ferromagnetism which implies a fundamental influence of the coordination and of local symmetry. On the other hand, with the shrinking dimensions of devices like high density magnetic memories the related phenomena become technologically more and more relevant. In this presentation experimental results on epitaxial ultrathin films and nanostructures

are discussed on the following aspects:
- enhanced ground state magnetic moments
- interface magnetic anisotropies
- spin excitations and phase transitions.

Characteristic changes are observed when the transition is made from bulk material to ultrathin films in the monolayer range and from extended films to artificially patterned dot arrays with sub-micrometer dot diameter. In particular, the magneto-crystalline anisotropy at an interface is affected by the reduced symmetry and coordination. In addition to the well-known out-of-plane surface anisotropy an in-plane interface anisotropy is found which shows a universal behavior and has the opposite sign compared to the respective volume anisotropy. It is demonstrated that this effect is exclusively determined by the specific lattice symmetry (bcc or fcc). Finally, it is shown that reduced dimensions significantly alter the spectrum and energies of spin excitations. Especially, continuously enhanced thermal spin excitations and a lowering of the Curie temperature, T_C, are observed when the film thickness is reduced to a few atomic layers and when a continuous film is patterned into circular dots with decreasing diameter. The effect of magnetic anisotropies on spin wave excitations and on T_C predicted by theory is discussed with respect to second order (uniaxial) and fourth order anisotropies.

MAGNETIC TUNNELJUNCTIONS MADE FROM HALF-METALS

Stefan Blügel

IFF, Forschungszentrum Jülich, D-52425 Jülich, Germany

Half-metallic ferromagnets are ferromagnetic materials showing, in the ideal case, 100% spin polarization at the Fermi level E_F, due to a metallic density of states in one spin direction (usually majority spin) combined with a band gap in the other spin direction (usually minority spin). In principle, half-metallic ferromagnets are ideal spin injectors and detectors, because under moderate voltage they can carry current in only one spin direction. Therefore, they also constitute ideal components for tunneling magnetoresistant (TMR) devices, with two half-metallic leads sandwiching a nonmagnetic semiconducting or insulating spacer. On the other hand, the tunneling current in these TMR devices is very small so that the conventional interpretation in terms of a Landauer-Büttiker picture of ideal interfaces are bound to fail. In this talk we emphasize that interface states at the interfaces of tunneljunctions can have severe implications on the tunnel-magnetoresistance ratio. We propose an antiferromagnetically coupled TMR element made of half-metals without interface state based on an *a priori* understanding of the exchange interactions in such systems, as a paradigm of materials design from first principles.

CORRELATIONS IN ELECTRONIC TRANSPORT THROUGH NANOSTRUCTURES

B.R. Bułka[1], **T. Kostyrko**[2] **and P. Stefański**[1]

[1] Institute of Molecular Physics, Polish Academy of Sciences,
ul. M. Smoluchowskiego 17, 60-179 Poznań, Poland

[2] Institute of Physics, A. Mickiewicz University,
ul. Umultowska 85, 61-614 Poznań, Poland

In devices of a nanoscale two phenomena play crucial role in electronic transport: coherent transmission and electronic correlations. Some recent results of coherent transport in a presence of strong electron correlations are presented. In particular we are interested in many-body effects, as the Kondo resonance. As an example a system with two quantum dots connected in series is considered, for which all many-electron correlation functions are determined for an arbitrary number of electrons. The studies predict a new feature in transport resulting from transmission through a triplet state, which can be activated for larger source-drain voltages. An analysis of the spin-spin correlation function allows an insight into formation of the total spin and its influence on transport. The quantum interference effect is also seen in the conductance through the double quantum dot. For a large quantum dot one can expect a discrete set of pointer states, which make conditions for the Fano resonance. Our theoretical results for the conductance are in good agreement with experimental measurements on semi-open quantum dots.

MAGNETIC PROPERTIES OF NONSTOICHIOMETRIC AND SUBSTITUTED $SrRuO_3$

B. Dąbrowski

Physics Department, Northern Illinois University, DeKalb, IL 60115, USA

$SrRuO_3$ has been known for half a century as a strongly-correlated ferromagnetic metal and proposed for use as an electrode material in micro- and nano-electronic circuits. We have discovere that annealing of stoichiometric $SrRuO_3$ perovskites in high-pressure oxygen produces $SrRu_{1-v}O_3$ compounds with vacancies on the Ru-sites. The creation of Ru vacancies rapidly suppresses ordered moment per Ru from 1.6 to 0.8 μ_B and the ferromagnetic ordering temperature, T_C, from 163 K to 45 K with increase of v $\approx$ 0.09, whereas the resistivity increases. Subtle structural changes that accompany creation of Ru-site vacancies are different from the typical properties of transition metal perovskites, for which an increased formal oxidation state of the B-site cations normally leads to decreased B-O interatomic distances and contraction of the unit cell volume. The reduced charge screening caused by the Ru-vacancies offsets expected decrease of the average interatomic distance Ru-O and rotation of the RuO_6 octahedra as Sr atoms relax toward Ru-vacancies increases observed volume. Local probes of Ru with XANES, NMR, and EELS find no valence change while isomer shifts of ^{99}Ru from Mössbauer experiments reveal a small change from +4 toward +5 as the T_C decreases.

By using "design rules" of the synthesis and magnetic interactions for perovskites we have establishe that Cr substitution into Ru site of $SrRuO_3$ increases T_C to 188 K at the solubility limit of 12% . The ^{53}Cr and ^{99,101}Ru NMR studies reveal that the electronic configurations of Cr and Ru are $3d^3$ ($t_{2g}^{3\uparrow}$) and $4d^4$ ($t_{2g}^{3\uparrow 1\downarrow}$), respectively. Compared with $SrRuO_3$, the spin-down electron in Ru 4d shell is more itinerant in $SrRu_{0.875}Cr_{0.125}O_3$ which is consistent with a broadened conduction band and a possible minority band $Cr(d^3)$-O^{2-}-$Ru(d^4)$ double-exchange-like interaction. The exchange interaction involves the Cr^{3+} into the ferromagnetic ordering

and enhances the ordering temperature. This picture is supported by a steady decrease of the ordered moment per Ru/Cr.

Neutron powder diffraction analysis revealed that below $T_c = 163$ K the b and c lattice parameters and the unit cell volume are virtually temperature independent for the stoichiometric material. We show that this previously reported invar-effect below the ferromagnetic ordering temperature originates from freezing of the octahedral tilting about the [001] axis. The invar-effect is much less pronounced in the Ru-deficient samples with decreased T_c 's = 135 K and 82 K. We show that the invar-effect gradually disappears also for the Cr-substituted samples with increased T_c 's.

Supported by the NSF-DMR-0302617 and by the US Department of Education

This research was conducted in collaboration with O. Chmaissem, S. Kolesnik, P.W. Klamut, S. Mini, Y. Ito, M. Maxwell, J. Mais, and T. Maxwell, Physics Department, Northern Illinois University, DeKalb, IL 60115, USA; J.D. Jorgensen, M. Avdeev, P. Barnes, and S. Short,

Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA; Z.H. Han, J.I. Budnick, and W.A. Hines, Department of Physics, University of Connecticut, Storrs, CT 06269, USA; M. De Marco, D. Coffey, and R. Heary, Physics Department, Buffalo State College, Buffalo, New York 14222, USA; S. Toorongian and M. Haka,Nuclear Medicine Department, State University of New York, Buffalo 14260, USA.

PERCOLATION EFFECTS IN DILUTE MAGNETIC SEMICONDUCTORS

Peter H. Dederichs* , ***K. Sato** and H. Katayama-Yoshida*** **

*Research Center Jülich, Germany, **Osaka University, Japan

We discuss the origine of ferromagnetism in dilute magnetic semiconductors with wide band-gaps such as (Ga,Mn)N or (Zn,Cr)Te as compared to the ferromagnetism in systems like (Ga,Mn)As or (In,Mn)As. While in the later case, the ferromagnetism is caused by Zener's p-d exchange, in systems like (Ga,Mn)N and (Zn,Cr)Te the main interaction is Zener's double exchange. The electronic structure calculations are performed by using the KKR-Green function method in connection with the CPA to describe the substitutional disorder of the transition metal atoms. We use both the local density approximation (LDA) and the LDA+U method to describe correlation effects. The exchange interaction constants Jij between two magnetic ions are calculated by embedding the two ions i and j into an effective CPA-medium. The Curie temperatures are calculated from the Heisenberg model by Monte Carlo simulations using Binder's cumulant method. The general trend for impurity band systems is, that the exchange interactions Jij are very strong, but short ranged. Therefore the interaction is dominated by a strong nearest neighbour interaction. This has important consequences. For instance, in dilute systems percolation of the strong nn interactions cannot be achieved, since the concentrations are far below the percolation threshold. Therefore the ferromagnetism is dominated by the weak longer-ranged interactions and the Curie temperatures are very low.

CHARGE-ORDERING FLUCTUATIONS AND ANOMALOUS RAMAN RESPONSE IN CUPRATES

C. Di Castro

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The stripe quantum critical point theory for high T_c superconductors was shown to imply various pseudogap-formation-temperatures with soft and hard pseudogaps, scaling form for optical conductivity and an anomalous isotope effect. We point out here that there is a direct contribution of charge collective fluctuations to the Raman spectra, which becomes a nice probe of the theory. We find that the critical charge collective modes can or cannot be excited depending on the direction of their wavevector and on the polarization of the incoming and outgoing photons. This provides a direct confirmation that the order associated to the quantum critical point near optimal doping of Cuprates occurs at finite wavevectors.

CARRIER-CONTROLLED FERROMAGNETIC SEMICONDUCTORS

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Recent advances in understanding of carrier-controlled ferromagnetism in tetrahedrally coordinated diluted magnetic semiconductors and their nanostructures will be reviewed with a focus on the phenomena important for prospective spintronic devices. Experimental results for III-V materials, where the Mn atoms introduce both spins and holes, will be compared to the case of II-VI compounds, in which the Curie temperatures T_C above 1 K have been observed for the uniformly and modulation-doped p-type heterostructures but not in the case of n-type films. The experiments demonstrating the tunability of T_C by light and electric field will be presented. The tailoring of domain structures and magnetic anisotropy by strain engineering and confinement will be discussed emphasizing the role of the spin-orbit coupling in the valence band. Recent progress in search for semiconductors with T_C above room temperature and hopes associated with compounds containing magnetic ions other than Mn will be presented.

This work is partially supported by ERATO Semiconductor Spintronics Project of Japan Science and Technology Agency, KBN grant, and Humboldt Foundation; for review, see, T. Dietl and H. Ohno, MRS Bulletin, October 2003, p. 714, and for recent preprints, T. Dietl et al., http://www.arxiv.org/find/cond-mat.

MAGNETISM IN MANGANITES AND MANGANITE-TITANATE BIFERROICS

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Ferro- or antiferromagnetic manganites (La,A)MnO_3 have been investigated mainly for two reasons during the last decade: First, the high spin polarization of conduction electrons in the conducting manganites might be useful in spintronics devices. Second, the competition of charge, orbital and lattice degrees of freedom leads to a variety of different ground states which are controllable by external parameters like magnetic or electric fields, pressure und lattice strain in thin films or light. In our work, epitaxial thin film systems of manganites and titanates ($SrTiO_3$ and ferroelectric $PbZr_{0.48}Ti_{0.52}O_3$ (PZT))have been prepared by the off-axis pulsed laser deposition (PLD) method that allows to grow coherently strained and smooth films. Investigations on tunnel trilayers of $La_{0.7}Ce_{0.3}MnO_3$-$SrTiO_3$-$La_{0.7}Ca_{0.3}MnO_3$ indicate the electron-doped and minority-carrier nature of the Ce-doped manganite. Epitaxial bilayers of a manganite and PZT show both, biaxial strain induced by the PZT inverse piezoelectric effect and an electrical field effect modulating the manganite carrier density near the interface. Additionally, piezoelectric substrates have been employed to reproducibly control the strain state of manganite films deposited on top. Data on electrical transport and magnetism of these biferroic thin film systems will be discussed.

RELATIVISTIC AND CORRELATION EFFECTS IN MAGNETIC SOLIDS

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The interplay of magnetic ordering and spin-orbit coupling leads to a large variety of phenomena that are even of great technological importance. Corresponding well known examples are the magneto-crystalline anisotropy or orbital contributions to the magnetic moments and hyperfine fields. As a peculiar spin-orbit induced ground state property one may add the occurrence of a field gradient in cubic ferromagnets. Besides the galvano-magnetic effects spin-orbit coupling in addition gives rise to many interesting effects in electron spectroscopy. A theoretical approach is presented that allows a detailed investigation of these spin-orbit induced phenomena in magnetic solids. This is achieved by using the spin-polarized relativistic version of multiple scattering or Korringa-Kohn-Rostoker (SPR-KKR) formalism on the basis of local spin density functional theory (LSDA). Corresponding applications to a variety of transition metal bulk, surface and cluster systems will be presented. To allow for a more detailed discussion of the results a simplified analytical approach will be used. As LSDA turns out to provide often an insufficient basis -in particular when dealing with magnetic properties connected with the orbital degree of freedom of an electron- various schemes that are designed to allow for an improved treatment of correlation effects will be presented together with corresponding results.

IN-PLANE MAGNETIC MICRO- AND NANOPATTERNS: FUNDAMENTALS, APPLICATIONS, AND POSSIBILITIES

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Ion bombardment in an external magnetic field has become an excellent tool to modify the magnetic properties of magnetic thin film systems showing the exchange bias effect. Additionally this novel technique enables lateral magnetic patterning of these layer systems without topography contrast. Magnetic patterns can be achieved either by focussed ion beam techniques or by combining lithography techniques with broad ion bombardment. To understand the fundamental effects of ion bombardment induced magnetic modifications in exchange bias layer systems, the involved modification processes will be discussed in the context of a tentative model. Some applications of ion bombardment induced magnetic patterning (IBMP) will be shown and some further application possibilities will be discussed.

MAGNETIZATION REVERSAL BY INJECTION AND TRANSFER OF SPIN: EXPERIMENTS AND THEORY

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The magnetization of a ferromagnetic body can be reversed without applying a magnetic field but only by transferring spins from a spin-polarized electrical current. A reversal can be obtained either by the coherent precession of the magnetic moment generated by the transfer of spin, or by the motion of domain walls induced by the spin-polarized current. In other conditions the magnetization can also be maintained in precession by spin transfer. This maintained precession generates oscillations of the current in the microwave frequency range. Several theoretical approaches, extending the initial theories (Slonczewski, Berger), have been recently developed. The first part of the lecture describes experiments of both types, that is current-induced reversal by coherent precession and current-induced domain wall motion. The first type of experiment is performed on F/N/F submicronic pillars fabricated by an e-beam lithography method (F = ferromagnetic metal or semiconductor, N = nonmagnetic metal or semiconductor). In the second type of experiments, the magnetic configuration of spin valves is switched by current-induced domain wall motion in the soft layer between two pinning centers. This type of current-induced magnetic switching, as it requires smaller current densities than the magnetization reversal in pillars and can also be obtained by very short current pulses, is promising for applications. In the second part of the talk, I summarize the theoretical issue and describe the model we have developed to unify the interpretation of CPP-GMR and spin transfer experiments on pillars. This

model is based on a self-consistent calculation of the longitudinal and transverse components of the spin current throughout the multilayered structure in the limit of quasi-interfacial spin transfer. The torques acting on the magnetic layers are derived from the transverse component of the spin current injected into each layer. I will also discuss the different behaviors expected in different ranges of applied field (direct reversal or maintained precession).

GaMnAs MATERIALS AND NANOSCALE DEVICES

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By careful control of MBE growth conditions and post growth annealing procedures we have produced GaMnAs epilayers which high conductivities and Curie temperature up to 173K. We demonstrate that the improvement in material properties resulting from annealing is due to the out diffusion of interstitial Mn (PRL **94**, 127202 (2005)) . We find that compensation is very low in best samples. We show that our measured Curie Temperatures, Hall conductivities and AMR are in good agreement with the mean field theory. We also find that there is no evidence of a fundamental magnetisation deficit in our material.

We also present the observation of a large tunneling anisotropic magnetoresistance (TAMR) in thin (Ga,Mn)As epilayers with lateral nanoconstrictions (PRL **92** 037201 (2004)). The observation establishes the generic nature of the recently discovered TAMR effect, which originates from spin-orbit coupling in a ferromagnet and is not specific to a particular tunneling geometry. The lateral geometry allows us to directly link normal anisotropic magnetoresistance (AMR) and TAMR. This indicates that TAMR may be observable in other materials showing room temperature AMR, and suggest a re-examination of previous tunneling and nanocontact results.

PROPAGATION, TUNNELING AND PHASE SHIFT OF SPIN WAVES AT A MAGNETIC FIELD INHOMOGENEITY

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We show experimentally and by numerical simulation, that spin waves propa-gating in a magnetic film can pass through a region of a magnetic field inho-mogeneity or, alternatively, can be reflected by this region depending on the sign of the inhomogeneity. If the region is reflecting and narrow enough, spin wave tunneling takes place. We investigate the tunneling mechanism and de-monstrate that it has a magnetic dipole origin. While travelling through a region of inhomogeneous field, spin waves undergo a phase shift. We show, that this can be used for designing phase shifters and spin-wave logic elements.

MAGNETISM AND CHARGE RESPONSE IN QUASI-1D WIGNER LATTICE COMPOUNDS

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Doped edge-sharing Cu-O chain compounds are ideal realizations of 1D Wigner lattices. Such doped edge-sharing chains are found in the recently synthesized $Na_3Cu_2O_4$ and $Na_8Cu_5O_{10}$ systems [1], and they are also structural elements in the widely studied composite compounds $Sr_{14-x}Ca_xCu_{24}O_{41}$. As a result of the geometrical structure (90 degree Cu-O-Cu coordination) the hopping matrix elements and hence the kinetic energy is small compared to the Coulomb energy. At low temperature the charge order resulting from Coulomb interaction $V_l \sim 1/l$ generates Heisenberg chains with varying distance between spins, i.e., dictated by the Coulomb interaction. We analyse the strikingly different magnetic properties of $Na_3Cu_2O_4$ and $Na_8Cu_5O_{10}$ adopting the picture of *modulated Heisenberg chains*. We discuss the role of quantum charge fluctuations on magnetism. Spin-charge coupling is manifested in the fluctuation of spin positions, which results in a doping dependence of exchange interactions.

In the final part, we turn to the charge dynamics of Wigner lattices. Charge excitations are described as fractionally charged domain walls in these systems. We present a detailed discussion of domain-wall excitation spectra, excitonic states, and of the temperature dependence of optical conductivity [2].

[1] P. Horsch et al., Phys. Rev. Lett. **94**, 076403 (2005).
[2] M. Mayr and P. Horsch, (to be published)

FRUSTRATED ANTIFERROMAGNETIC QUANTUM CHAIN SYSTEMS

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Antiferromagnetic (afm) S=1/2 Heisenberg chain systems with uniform nearest-neighbour exchange coupling are best understood. The ground state and the excitation spectrum are well known and the experimental observations are in good agreement with theory. Additional next-nearest neighbour exchange along the chains which can be described by the Majumdar-Ghosh Hamiltonian $H = J_{nn} \sum_i (S_i S_{i+1} + \alpha S_i S_{i+2})$ with α=J_{nnn}/J_{nn} gives rise to a more complex behaviour, since next-nearest neighbour interaction may lead to magnetic frustration. I review the magnetic properties of the afm S=1/2 Cu^{2+} chain systems $LiCuVO_4$ and CuX_2 (X=Cl, Br) for which afm *incommensurate* long-range ordering has been observed by neutron diffraction at low temperatures. The appearance of incommensurate ordering is ascribed to competing *nn* and *nnn* exchange interaction which is also evidenced in the bulk magnetic properties.

SPIN-CHARGE SEPARATION AND NON-LINEAR OPTICAL RESPONSE IN ONE-DIMENSIONAL CUPRATES

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The spin-charge separation is one of the key concepts in strongly correlated electron systems in one-dimension[1]. This also provides an opportunity for much debate on high temperature superconductivity. The Mott gap, i.e., the charge excitation gap in strongly correlated electron systems is in contrast to the energy gap in band insulators. Recent experiments have revealed that Mott insulators in one-dimension exhibit the strikingly large non-linear optical response. Here, we theoretically examine the spin-charge separation and the linear and non-linear responses in one- dimensional Mott insulators and clarify the nature of the photo-excited states. In particular, we focus on the followings: (i) the linear absorption which is characterized by the odd-parity excited states, (ii) the two-photon absorption (TPA) which is characterized by the even-parity excited states, and (iii) the third-harmonic generation (THG). The theoretical results are compared with the experimental ones. We discuss the similarity and dissimilarity of the electronic and optical properties in one- and two-dimensional Mott insulators based on the spin-charge separation.

This work has been done in collaboration with T.Tohyama, H.Matsueda, N.Bulut. [1] S. Maekawa et al.: *Physics of Transition Metal Oxides* (Springer, 2004)

D-WAVE DENSITY WAVES IN HIGH T_C CUPRATES AND $CeCoIn_5$

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As is well known there are many parallels between high T_c cuprate superconductors and heavy fermion compound $CeCoIn_5$; quasi two dimensional Fermi surfaces, vicinity of antiferromagnetism and d-wave superconductivity. Recently giant Nernst effect and angle dependent magnetoresistance (ADMR) are observed in the pseudogap phases in both high T_c cuprates and $CeCoIn_5$. We shall describe these phenomena in terms of d-wave density waves. Also some properties of the gossamer superconductivity (d-wave superconductivity in the presence of d-wave density wave) will be explored.

NEW SPIN CONFIGURATIONS IN NANO-SIZED MAGNETS NEAR REORIENTATION PHASE TRANSITION

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By micromagnetic simulations and analytically we study the ground and metastable magnetic states of ultrathin magnets (with thickness d) in the form of films and laterally size-limited samples: semi-infinite films, wires (width w) and disks (radius r). Nanostructures are discussed with low-perpendicular magnetic anisotropy determined by the quality factor Q - the ratio between magnetic anisotropy and demagnetization energies. Simulations are based on real material parameters, determined for ultrathin Co with defined Q(d) dependence. Domain structure existence decrease Q when the transition into in-plane phase undergoes down to $Q^* < 1$ [1]. Out-of-plane magnetization component exists at the edge of semi-infinite film when $Q > Q_{edge}$ ($Q_{edge} < Q^*$). Perpendicular magnetization states can be achieved by properly decreasing lateral nanostructure size in whole Co ultrathin thickness regime. Q dependent different scenarios of magnetization distribution changes decreasing parameters w or r are discussed for nanostructure with defined d. Novel nanometer-scale magnetization distributions are discussed such as: domain-like distribution with an oscillating out-of plane magnetization component and decaying amplitude; out-of plane component patterned vortex.

[1] M. Kisielewski et. al., Phys. Rev. B (2004) **69**, 184419.

MAGNETIC AND SUPERCONDUCTING CORRELATIONS IN THE 2D HUBBARD MODEL

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The functional renormalization group (fRG) is an ideal tool for dealing with the hierarchy of energy scales and competition of different interactions in correlated electron systems. Starting point is an exact hierarchy of flow equations which yields the gradual evolution of the effective low-energy action from the microscopic model Hamiltonian as a function of a continuously decreasing energy cutoff. Truncated at one-loop level the fRG yields a systematic and unbiased weak coupling stability analysis, where the competition and mutual feedback of particle-particle and particle-hole channels is consistently taken into account. The latter channel drives in particular magnetic, the former superconducting correlations. For the weakly interacting 2D Hubbard model detailed information on the dominant low-energy effective interactions and correlations has been obtained from numerical solutions of the one-loop flow equations. These calculations conclusively established the existence of d-wave superconductivity in the 2D Hubbard model at weak coupling. In a regime with strong antiferromagnetic correlations the spectral function for single-particle excitations obtained from the two-loop self-energy exhibits pseudogap features near van Hove points or other hot spots on the Fermi surface.

MAGNETIC MICROSTRUCTURE OF NANOPERM-TYPE NANOCRYSTALLINE ALLOYS

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A brief description of the influence of structural modifications caused by temperature of annealing (i.e. number of nanocrystallites) as well as by temperature of measurement upon magnetic behaviour of nanocrystalline alloys of the NANOPERM family prepared from amorphous precursors will be given. Results of nuclear and atomic based techniques of (subatomic) structural characterization comprising Mössbauer spectrometry, XRD, TEM, HREM, DSC, and AFM will be correlated with magnetic data obtained from macroscopic measurements.

DOPED 2D FRUSTRATED QUANTUM MAGNETS: SPIN-CHARGE SEPARATION AND NON-CONVENTIONAL SUPERCONDUCTIVITY

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Dynamics of mobile holes in two-dimensional frustrated quantum magnets is investigated. Numerical evidences are provided for spin-charge separation under doping the Kagome lattice, a featureless spin liquid. On the contrary, in the checkerboard lattice, a candidate of broken-symmetry Valence Bond Crystal, a small quasi-particle weight exists for some crystal momenta, a finding interpreted as a restoration of weak holon-spinon confinement (1). Amplification of pairing occurs in this case (for $t > 0$) due to a localisation process that blocks single hole tunneling between the plaquettes of the Valence Bond Solid while hole pairs can delocalize (2). This scenario can give rise to new singlet pairing channels with s-, d- or g-wave symmetries. I also argue that the formation of a spatially-extended region where the plaquette solid melts around the hole can lead to an effective correlated hopping responsible for the two hole boundstate.

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MAGNETIC EXCITATIONS IN MAGNONIC CRYSTALS AND IN SMALL MAGNETIC PARTICLES

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Magnetic normal modes, vital for the problem of thermal noise in small magnetic elements used in writing/reading devices, are investigated here in finite thin films, cube grains and rods. We show how a strong inhomogeneity of the demagnetizing field in these structures induces amplitude bulk localization of magnetostatic modes. Moreover, a new type of magnetostatic modes (*comb modes*) is found in a spectrum of elongated axially magnetized rods, with two clearly discernible

regions: a zone of fast amplitude oscillations inside the rod, and slow-oscillation narrow regions at the borders. Absorbing virtually no energy from an *applied* alternating field, comb modes have no significant contribution to the magnetic noise. A separate issue to be raised in this study is that of magnetic excitations propagating in *magnonic crystals* (MC), *i.e.* hypothetical macrocrystals with periodically inhomogeneous magnetic structure, topologically equivalent to well known photonic crystals [1]. Magnonic spectra are investigated in 1D, 2D and 3D structures, and conditions of opening of energy gaps forbidden to magnonic propagation are determined in particular. A confrontation of our 3D MC theory with recent experimental results (spin-wave spectra measurements through neutron scattering) obtained in certain low-doped manganites allows us to suggest a hypothesis that these materials can be regarded as magnonic crystals *existing in nature*.

[1] H. Puszkarski, M. Krawczyk, "Magnonic Crystals - the Counterpart of Photonic Crystals", Solid State Phenomena, **94**, 125 (2003) and references therein.

MAGNETIC PROPERTIES OF ALMOST LOCALIZED FERMIONS - REVISITED

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The properties of almost localized fermions became a subject of a renewed interest in recent years. This is caused by the discovery of the spin-dependent heavy masses predicted some time ago [1] as well as of critical behavior near metal-insulator transition of the Mott-Hubbard type [2]. We discuss these properties within our earlier approach [3] and include the quantum Gaussian fluctuations. A strong metamagnetic behavior is connected to the spin-dependent masses. Effect of the orbital degeneracy on these effects is also briefly mentioned within an original rotationally invariant version of the extended Hubbard model containing the Hund's rule coupling.

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R. Citro et al., Physica B **261**, 213 (1999).
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[3] J. Spałek and W. Wójcik, in *Spectroscopy of the Mott Insulators and Correlated Metals*, Springer Tracts in Solid State Sciences **119**, pp. 41-65.

UNCONVENTIONAL FORMS OF SUPERCONDUCTIVITY AND QUANTUM CRITICALITY IN HEAVY-ELECTRON METALS

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Some recent observations made on the isostructural compounds $CeCu_2Si_2$ and $YbRh_2Si_2$ are discussed. We first address the interplay of superconductivity in $CeCu_2Si_2$ with both a spin-density-wave-type quantum critical point (QCP) at low pressure [O. Stockert et al., PRL **92**, 136402 (2004)] and a weak valence transition of Ce at high pressure [H. Q. Yuan et al., Science **302**, 2104 (2003)]. We then turn to $YbRh_2Si_2$ displaying a novel type of QCP [J. Custers et al., Nature **424**, 524 (2003); S. Paschen et al., Nature **432**, 881 (2004)], which appears to be detrimental to superconductivity.

Work done in collaboration with:
J. Custers, P. Gegenwart, C. Geibel, F. M. Grosche, R. Küchler, K. Neumaier, S. Paschen, J. Sichelschmidt, G. Sparn, Y. Tokiwa, H. Wilhelm, S. Wirth, H.Q. Yuan, P. Coleman, C. Pépin, Q. Si and G. Zwicknagl

RENORMALIZATION GROUP APPROACH TO WEAKLY INTERACTING SPIN AND FERMION CHAINS

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The properties of many real materials are dominated by the presence of weakly coupled chains. We propose a method based on the real space renormalization group transformation which can be used to study critical behavior and thermodynamics of a broad class of the weakly interacting classical and quantum spin chains with $S \geq 1/2$ in an magnetic field as well as fermion chains. The method is presented and examined for the standard Ising model on a rectangular lattice and then applied to the weakly interacting quantum anisotropic Heisenberg model and spinless fermion system. We discuss a dimensional crossover in coupled spin chains. We also show that the characteristic feature of a strongly correlated spinless fermion chain is a double peak structure of the specific heat as a function of temperature and a small interchain (transverse) hopping leads to a phase transition from a metallic to a charged ordered phase.

SUPERFLUIDITY IN CONDENSED EXCITONS BELOW 20 K

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In superconductivity the electrical conductivity is diverging at the critical temperature, in superfluidity the heat conductivity is diverging. Therefore, the measurement of heat conductivity and thermal diffusivity is giving the essential information if superfluidity occurs. Superfluidity needs a "fluid" to start with and in a solid this means a condensed state of bosons. Such bosons are Coulomb coupled electron-hole states, excitons, which can condense. In materials, which exhibit intermediate valence, 4f holes can be very heavy with masses around $100\,m_e$ and, nevertheless, the compounds can be narrow gap semiconductors. Such a material is $TmSe_{0.45}Te_{0.55}$

and its thermal properties have been measured as function of temperature (4 K) and pressure (17 kbar). Below 20 K the heat conductivity and the thermal diffusivity diverge exponentially with decreasing temperature, being indicative of superfluidity. Above this temperature the condensed excitons can order in a Wigner lattice, couple to phonons, and thus, creating exciton-polarons with very anomalous specific heat and sound velocities with a special dispersion. For the first time stable exciton condensation with permanent superfluidity has been observed.

PHYSICS OF NANOMAGNETISM REVEALED BY SPIN-POLARIZED SCANNING TUNNELING SPECTROSCOPY

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n order to probe and tailor magnetic properties at the spatial limit we have combined the scanning tunneling microscope (STM) with spin-sensitivity [1-3]. This is achieved by the use of ferro- [4-6] and antiferromagnetically [7, 8] coated probe tips offering a high degree of spin-polarization of the electronic states involved in the tunneling process. Spin-polarized Scanning Tunneling Microscopy (SP-STM) and Spectroscopy (SP-STS) has allowed the visualization of atomic-scale spin structures [2, 9] and the investigation of the spin-dependent local density of states spatially resolved [10]. Magnetic domain imaging with sub-nanometer-scale spatial resolution has been demonstrated for magnetic transition metal as well as rare earth metal films. Ultra-sharp domain walls were discovered in ultra-thin iron films on W(110) substrates [11]. In a recent SP-STM experiment we could prove that single monolayers of Fe on W(001) substrates exhibits a c(2x2) antiferromagnetic ground state with perpendicular anisotropy in contrast to a single Fe monolayer on W(110) which is ferromagnetic with in-plane anisotropy [12]. Spin-dependent scattering at single oxygen impurities on Fe/W(110) was visualized in real-space reflecting the orbital nature of the electronic states involved as well as their spin character [13]. Finally, applications of SP-STM for studying spin states of single magnetic impurities will be discussed.

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GIANT ROOM-TEMPERATURE TMR EFFECT IN MAGNETIC TUNNEL JUNCTIONS WITH MgO(001) TUNNEL BARRIER

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Magnetic tunnel junctions (MTJs) consisting of ferromagnetic electrodes separated by a tunnel barrier exhibit the tunneling magnetoresistance (TMR) effect. While a magnetoresistance (MR) ratio up to 70% has been obtained at room temperature (RT) in MTJs with an amorphous Al-O tunnel barrier, a much higher MR ratio is theoretically expected in fully-epitaxial MTJs with a crystalline MgO(001) tunnel barrier. We fabricated the fully epitaxial Fe(001)/MgO(001)/Fe(001) MTJs with MBE and micro-fabrication techniques and achieved a giant MR ratio up to 188% at RT.[1,2)] We observed even higher MR ratio up to 271% at RT (353% at 20 K) in fully-epitaxial bcc Co(001)/MgO(001)/Fe(001) MTJs. We also fabricated MTJs consisting of a highly-oriented poly-crystalline MgO(001) barrier and amorphous CoFeB ferromagnetic electrodes with sputtering deposition technique.

The CoFeB/MgO(001)/CoFeB MTJs also exhibited a giant TMR effect above 200% at RT.[3)] A crystalline MgO(001) tunnel barrier seems to be essential for the giant TMR effect because an amorphous MgO tunnel barrier yielded a much lower MR ratio. These results are of great importance not only for industrial applications but also for the physics of spin-dependent tunneling.

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2.1.2 Report on Hands-on Course "KKR Bandstructure and Spectroscopy Calculations"

München, 9-11 June 2005

A hands-on course on the KKR method entitled "KKR Bandstructure and Spectroscopy Calculations" took place in München 9-11 June 2005. It welcomed 28 participants and 20 lecturers (the list of participants and lecturers is given below).

The aim of the workshop was to introduce new users from theory as well as experiment into the Munich SPR-KKR (spin polarized relativistic Korringa-Kohn-Rostoker) program package (see http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR/). The highly automated program package not only allows to study the electronic structure of solids by calculating bands, densities of states, total energies etc, but also gives access to the calculations of many spectroscopic properties as probed for example by XANES, EXAFS, magneto-optics, angle integrated photoemission, Auger electron spectroscopy or Compton scattering. The codes can be run in a non-relativistic and relativistic manner and contain several tools to analyse the effect of the spin-orbit interaction. Moreover, the package can treat ordered and disordered alloys and magnetic multilayers. In addition, the package supplies many tools to analyse the electronic structure such as wave function, phase shift or matrix element plots. All of this was embedded into an easy to use multi purpose Graphical User Interface (GUI) called XBAND (see http://olymp.cup.uni-muenchen.de/ak/ebert/xband.html), that can easily be adopted to support other bandstructure packages. Set exercises for three afternoons were prepared to give the participants the opportunity to acquaint themselves with all features of performing electronic structure and spectroscopy calculations. In addition, the participants were also given the opportunity to investigate systems of their own interest together with their spectroscopic properties.

A series of lectures accompanied the practical hands-on sessions. Nearly all lecture notes can be found under:
http://olymp.cup.uni-muenchen.de/ak/ebert/Handson_2005/. The fundamentals of the KKR method were taught by W. Temmerman and Z. Szotek. The relativistic version of the KKR and its implementation in the Munich SPR-KKR package were introduced by H. Ebert. The calculation of spectroscopic properties using the program package was demonstrated by J. Minar. As recent applications results on the high-field susceptibility of ferromagnetic metals, ferromagnetic clusters at finite temperature and free transition metal clusters were presented by S. Mankovskyy, S. Polesya and O. Sipr, respectively. In addition, there were invited theoretical talks: P. H. Dederichs dealt with diluted magnetic semiconductors and A. Soldatov reported on his work on XAFS of small nanoclusters. These presentations were complemented by invited talks given by experimentalists: H. Wende dealt with XAS of light 3d elements as a benchmark for ab initio calculations, K. Baberschke also addressed the relationship of experiment and theory concerning the magnetism of 3d monolayers grown with oxygen surfactant, J. Schmalhorst demonstrated the power of soft X-ray spectroscopy to investigate the interface structure and

magnetism of magnetic tunnel junctions with Heusler alloy electrodes and W. Warth reported on investigations of the magnetic properties of deposited transition metal clusters by using X-ray spectroscopy.

In addition, many participants presented poster contributions that led to lively discussions during the coffee breaks.

The large number of participants (not all applications could be accepted because the limited number of tutors and available computers), in particular with an experimental background, reflects the need for hands on courses introducing also non-experts to the field. The course in Munich surely succeeded in teaching the participants the basics of the rather complex KKR formalism as well as the use of the very user-friendly Munich SPR-KKR package.

Speakers:

H. Ebert	München	The Munich SPRKKR package
J. Minar	München	Calculating spectroscopic properties with the Munich SPRKKR package
H. Wende	Berlin	XAS of light 3d elements: a benchmark for ab initio calculations
P. H. Dederichs	Jülich	Diluted magnetic semiconductors
S. Mankovsky	München	High-field magnetic susceptibility of ferromagnetic metals
S. Polesya	München	Ferromagnetic clusters at finite temperatures
A. Soldatov	Rostov State University	XAFS of small nanoclusters
K. Baberschke	Berlin	New magnetism of 3d monolayers grown with oxygen surfactant: Experiment vs. ab initio calculations
W. M. Temmerman	Daresbury	KKR-basics I
J. Schmalhorst	Bielefeld	Magnetic tunnel junctions with Heusler alloy electrode: Interface structure and magnetism explored by soft X-rays
O. Sipr	Prague	Free clusters
W. Wurth	Hamburg	Magnetic properties of deposited transition metal clusters from x-ray spectroscopy
Z. Szotek	Daresbury	KKR-basics II

Invited speakers and tutors

Baberschke, Klaus – Institut für Experimentalphysik, FU Berlin, Germany
Benea, Diana – Ludwig-Maximilians-Universität München, Germany
Bornemann, Sven – Ludwig-Maximilians-Universität München, Germany
Chadov, Stanislav – Ludwig-Maximilians-Universität München, Germany
Dederichs, P.H. – Forschungszentrum Jülich GmbH, Jülich, Germany

Ebert, Hubert – Ludwig-Maximilians-Universität München, Germany
Kardinal, Marianne – Ludwig-Maximilians-Universität München, Germany
Ködderitzsch, Diemo – Ludwig-Maximilians-Universität München, Germany
Kosuth, Michal – Ludwig-Maximilians-Universität München, Germany
Mankovsky, Sergey – Ludwig-Maximilians-Universität München, Germany
Minar, Jan – Ludwig-Maximilians-Universität München, Germany
Polesya, Svetlana – Ludwig-Maximilians-Universität München, Germany
Popescu, Voicu – Ludwig-Maximilians-Universität München, Germany
Schmalhorst, Jan Michael – University of Bielefeld, Bielefeld, Germany
Sipr, Ondrej – Institute of Physics AS CR, Praha, Czech Republic
Soldatov, Alexander – Rostov State University, Faculty of Physics, Rostov-Don, Russia
Szotek, Zdzislawa – Daresbury Laboratory Daresbury
Temmerman, Walter – Daresbury Laboratory Daresbury
Wende, Heiko – Insitut für Experimentalphysik, Freie Universität Berlin, Germany
Wurth, Wilfried – Institut für Experimentalphysik, Hamburg, Germany

List of participants

Antoniak, Carolin – Universität Duisburg-Essen, Germany
Aziz,Bekhit, Emad Flear – BESSY GmbH, Berlin, Germany
Batt, Gary – Bristol University, UK
Bauer, Matthias – Inst. f. Physik. Chemie, Univ. Stuttgart, Germany
Belhadji, Brahim – Forschungszentrum Jülich GmbH Jülich
Däne, Markus – Martin Luther University, Halle, Germany
Emtsev, Konstantin – Institute of Technical Physics, University Erlangen-Nuremberg, Germany
Fecher, Gerhard H. – Johannes Gutenberg - Universität, Mainz, Germany
Flege, Jan Ingo – University of Bremen, Bremen, Germany
Go, Anna – Institute of Experimental Physics, University of Bialystok, Poland
Goraus, Jerzy – University of Silesia, Katowice, Poland
Johal, Tarnjit – CCLRC Daresbury Laboratory, Daresbury, UK
Kandpal, Hem – University Mainz, Mainz, Germany
Laverock, Jude – University of Bristol, UK
Lueders, Martin – Daresbury Laboratory, UK
Mouketo, Landry – The Abdus Salam ICTP, Trieste, Italy
Müller, Martina – FZ Jülich, Jülich, Germany
M'Passi-Mabiala, Bernard – The Abdus Salam ICTP, Trieste, Italy
Olimov, Khusniddin – Physikalisches Institut, Bonn, Germany
Rowlands, Derwyn – University of Bristol, Bristol, UK
Saha, Kamal – Max Planck Institute of Microstructure Physics Theory Department, Halle (Saale), Germany
Sahnoun, Mohammed – Department of Chemistry, University of Fribourg, Switzerland
Tallarida, Massimo – BTU Cottbus, Germany

Umeno, Yoshitaka – Institut fuer Zuverlaessigkeit von Bauteilen und Systemen (IZBS), Uni Karlsruhe, Germany
Welter, Edmund – HASYLAB at DESY, Hamburg, Germany
Winkelmann, Aimo – MPI für Mikrostrukturphysik, Halle, Germany
Zenia, Hand – Daresbury Laboratory, UK
Zhang, LingFei – University of Salford, Institute for Materials Research, UK

Abstracts

Molecular Structure of NaCl Electrolytes of Varing Concentration

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New magnetism of 3d monolayers grown with oxygen surfactant: Experiment vs. ab initio calculations

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Surfactant assisted growth of nanoscale structures on surfaces is a well established technique. Moreover, it is known that for ultrathin films of Fe, Co, and Ni the magnetic properties are highly sensitive to minimal structural changes: If the nearest neighbour distance varies by 0.03-0.05 $\AA$, only, the magnetic anisotropy energy (MAE) may change by 102-103. So the question arises: Can the growth of ultrathin 3d ferromagnets on single crystal substrates be manipulated using oxygen as a surfactant, or will an antiferromagnetic metal oxide be formed? The answer is threefold: i) We could indeed show by MEED and XAS that the growth is improved up to ¿20 ML and that finally the O atoms "float" on top of the ferromagnetic film (Surf. Sci. **566-568**, 100, *ibid* **565**, 197 (2004)). ii) Recent measurements demonstrate that the magnetic anisotropy energy is significantly enhanced using surfactants. Theory reveals that this is mainly due to the decrease in the magnitude of the surface anisotropy (PRL **92**, 147202 (2004)). iii) Preliminary experiments show that the chemisorbed oxygen atoms on the surface of the ferromagnetic film carry an induced magnetic moment.
The experiments will be discussed in context with ab initio calculations from the groups at Uppsala, Vienna, LMU and UCI.

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Comparative studies of methods for calculating the Fermi Surface of random metallic alloys

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We report on a comprehensive study of the similarities and differences between Molecular CPA [1] and the recently developed Non Local CPA [2] methods for calculating the electronic structure of random metallic alloys (solid solution). In particular we investigate their predictions for the Bloch spectral functions and effective Fermi surface. Furthermore we study the solution of the Fermi surface with bond filling and short ranged chemical order. Our results will be illustrated by explicit calculation based on a one band two dimensional tight-binding model.

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EXAFS/XANES Investigations into the Fe(III)-catalyzed Michael addition Reaction

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The Michael reaction of 1,3-dicarbonyl compounds with α,β-unsaturated carbonyls like methyl vinyl ketone is catalysed by Iron(III) salts under mild conditions with remarkable efficiency. Using $FeCl_3$ $6H_2O$ and $Fe(ClO_4)_3$ $9H_2O$ the disadvantages of traditional catalysts like Brönsted bases such as side and subsequent reactions can be avoided. In addition the environmentally friendly and cheap catalysts do not require special reaction conditions and no solvent is needed. The mechanism for this reaction has been proposed.

In this contribution we focus on the first step of the reaction cycle. The nature of complex 1 formed by dissolving $FeCl_3$ $6H_2O$ or $Fe(ClO4)_3$ $9H_2O$ in the β-keto ester Ethyl 2-oxocyclopentanecarboxylate (EOP) is so far unknown. Experimentally $FeCl_3$ $6H_2O$ shows a reduced catalytic activity compared to $Fe(ClO_4)_3$ $9H_2O$. Additionally the catalytic activity of $Fe(ClO_4)_3$ $9H_2O$ is reduced when Cl^- ions are added to the reaction mixture. Calculations in the gas phase predict binding of the chloride ions to the iron centre resulting in a reduced ability of the iron to coordinate ester molecules. To provide experimental proof, EXAFS and XANES-spectra of 2 mol% solutions of $FeCl_3$ $6H_2O$ and $Fe(ClO_4)_3$ $9H_2O$ in EOP were recorded together with several references and were analyzed with special focus on the coordination geometry of the iron centre by pre-peak evaluation.

The Munich SPR-KKR code

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The talk gives a short introduction to the functionality and formal background of the Munich spin-polarised relativistic (SPR-KKR) program package (see http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/SPRKKR/). First, in short the various available calculation modes, the electron structure information that can be obtained and the various kinds of electronic spectroscopy that can be studied are surveyed. Presenting the formal background of the SPR-KKR package emphasise is laid on the fully relativistic mode for magnetic solids. Technical details connected with that as for example the coupled radial Dirac equations, the single site t-matrix, symmetry considerations are discussed in some detail. Two ways to determine the so-called scattering path operator are explained: The real space cluster mode is used for high energies (EXAFS) and to deal with surfaces at the moment. The Brillouin zone integration technique, on the other hand, is used as the standard method for most other purposes. Using this technique exploiting symmetry is indispensable. The simultaneous presence of spin-orbit coupling and spin magnetisation, however, has rather important consequences for this as it is demonstrated. An important feature of the program package is the ability to deal with disordered systems by using the CPA (Coherent Potential Approximation). The basic ideas of he CPA are described and its implementation within the KKR-method is outlined. Finally, a short outlook on future developments is presented.

Electronic properties of clean unreconstructed 6H-SiC(0001) surfaces studied by angle resolved photoelectron spectroscopy

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The properties of the clean and unreconstructed SiC(0001) and SiC(000-1) surfaces were investigated by means of angle-resolved ultraviolet photoelectron spectroscopy. The measurements were conducted at the synchrotron light source BESSYII using a newly designed spectrometer of toroidal geometry (TEA) allowing us to collect all emission angles in one azimuthal plane simultaneously.

The clean, unreconstructed surfaces were prepared by exposing hydrogen terminated surfaces to a high flux of synchrotron radiation. Earlier findings on Si-rich $(\sqrt{3} \times \sqrt{3})$R30^o and (3x3) reconstructed surfaces of SiC show an interesting behavior in that the dangling bond surface bands undergo a Mott-Hubbard metal-insulator transition. The question addressed in this report is whether 11 unreconstructed SiC(0001) surfaces are still in the Mott-Hubbard regime or whether they exhibit the metallic surface suggested by theoretical calculations that don't take correlation effects into account.

First of all, valence band spectra show no states at the Fermi level before and after irradiation, that is, clean surfaces are semiconducting. Second, for Si and C terminated surfaces irradiation results in the appearance of the dangling bond states ≈0.8eV above, and close to the valence band maximum, respectively. These states lie in the gap of the projected bulk band structure. The bandwidth amounts to 0.2 and 0.6 eV for Si and C dangling bonds, respectively. Hydrogen desorption is accompanied by the disappearance of H-induced states in the valence band. Except for the location of the dangling bond band the electronic structure of the clean unreconstructed surfaces agrees with the existing band structure calculations. Therefore, clean unreconstructed Si- and C-truncated surfaces of 6H-SiC surfaces represent further examples of a Mott-Hubbard insulating surface despite a separation of the dangling bonds that is markedly reduced in comparison with the reconstructed surfaces.

Photon-stimulated Desorption and X-ray Standing Waves

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X-ray standing waves (XSW) using electrons and fluorescence photons as secondary signals have become a standard technique to determine adsorbate structures. However, when a sample is irradiated by intense light, desorption of ions is also a frequently observed phenomenon that is known as photon-stimulated desorption (PSD). But this signal is of a fundamentally different physical nature. The identification of this process has been a persistent topic in surface science throughout the last decades. By virtue of the inherent periodic time structure of synchrotron radiation, an efficient detection of positive ions emitted from the surface is feasible using time-of-flight spectroscopy. In this review, we will survey the relevant desorption mechanisms which initiate the prevailing processes. We will show that the combination of X-ray standing waves with X-ray PSD (XPSD) is a unique tool to identify the underlying desorption processes in a site-specific manner. In the contribution we will deal with the systems Si(111)-(7 x 7), H/Si(111)-(1 x 1), Ge/Si(111)-(1 x 1):H, and Cl/Si(111). This choice serves to illustrate the peculiarities of the different kinds of desorption processes and to demonstrate the general approach to the interpretation of XSW-XPSD data.

Site preference of manganese in $Fe_{3-x}Mn_xAl$ alloys

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A lot of attention has recently been paid to understand the fascinating structural and physical properties of iron aluminides that arise when some Fe atoms are substituted by other transition-metal atoms. Intermetallic compound Fe_3Al is a ferromagnet with DO_3-type crystal structure. The crystal lattice can be described as four interpenetrated face-centred cubic Bravais lattices originated at (0,0,0), (1/4,1/4,1/4), (1/2,1/2,1/2) and (3/4,3/4,3/4), and abbreviated as A, B, C and D, respectively. In the perfectly ordered structure there are two non- equivalent iron sites with different chemical neighbourhood - (A,C) and B sublattices. As a consequence different electronic and magnetic properties connected with these positions are observed as well as different site preferences depending on the element substituting for iron take place. According to Mössbauer and electron spectroscopy the doping manganese atoms have been found to occupy B sublattice [1]. However, nonempirical studies indicate that for x=0.2 manganese atoms preferentially occupy (A,C) sublattice and does not show any site preference for the lower of the considered concentrations [2]. The aim of our research is to investigate the site preference of atoms in compound $Fe_{3-x}Mn_xAl$ where iron is substituted by manganese. Results of the calculations carried out with the SPRKKR method [3] with the experimental values of the lattice parameter [4] are presented.

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Electronic structure of Ce2Rh3Al9

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Ce2Rh3Al9 is an interesting compound, known to possess mixed valence properties and unusual temperature dependence of resistivity. We have measured specific heat, electrical resistivity, magnetical susceptibility and XPS spectra of that compound. Moreover we calculated DOS by means of FP-LAPW and TB-LMTO-ASA method. Both methods predict pseudogap located on Fermi level. FP-LAPW result in half-metalic and LMTO in non-magnetic character of this compound. In low temperature resistivity, however, we do not see activated part, our explanation is that due to atomic disorder the gap is destroyed. Magnetical measurements don't show any ordering down to 2K, therefore the LMTO calculations seems to depict better the properties of that compound. Agreement between measured valence band spectra and calculated one is also quite good.

Calculated electronic structure of X_2YZ Heusler compounds

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Half metallicity has long been predicted using band structure method in the half Heulser NiMnSb and some other materials. More recently, certain full Heusler alloys have been predicted to show half metallicity. In this work, we present calculations on a series of X_2YZ full Heusler compounds which show the phenomenon of half metallic ferromagnetism. The crystal structures have been obtained for some of the compounds through structural relaxation in the first principles framework determining the minimum total energy as function of the lattice parameter. We find that mostly Co based Heusler compounds are exhibiting half metallic behaviour. We also analyze the influence of the lattice parameter on the minority band gap. We find that smaller lattice parameter result in larger minority band gaps. The width of the gap is seemingly a linear function of the lattice constant. X=Co based Heusler compounds exhibit high Curie temperature with a linear dependence on the number of valence electrons. Our results show that Co based Hesuler compounds obey the Slater-Pauling rule, while most of the others do not. There are slight changes in the magnetic moment of the Co atoms, while the magnetic moment of Y increases with the number of valence electrons. The pecularities of the electronic structure suggest that the Co based Heusler compounds are the best candidates for various spintronics applications.

Fermi surface nesting and charge-density-wave order in rare earth tri-tellurides

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The Fermi surface of rare-earth tri-tellurides ($R\mathrm{Te}_3$) is investigated in terms of the nesting driven charge-density wave formation using positron annihilation and first-principles LMTO calculations. Fermi surface nesting is revealed as a strong candidate for driving charge-density wave formation in these compounds. The nesting vector obtained from positron annihilation experiments on GdTe_3 is determined to be $\mathbf{q} = (0.28 \pm 0.02, 0, 0)\ \mathbf{a}^*$, ($\mathbf{a}^* = 2\pi/\mathbf{a}$), in excellent agreement with previous experimental and theoretical studies.

Self-interaction correction (SIC) in multiple-scattering theory

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We present applications of the Layer-KKR method, including the coherent potential approximation (CPA) to the calculation of the electronic structure and the photocurrents of magnetic

multilayers. We discuss how the photo-emission calculations can help to analyse experimental spectra. We present photo-emission spectra of quantum well systems. Furthermore we report on calculations of the magnetic moments of ultrathin films of Ni and V.

Self-interaction correction (SIC) in multiple-scattering theory

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We propose a simplified version of self-interaction corrected local spin-density (SIC-LSD) approximation, based on multiple scattering theory, which implements self-interaction correction locally, within the KKR method. The multiple scattering aspect of this new SIC-LSD method allows for the description of crystal potentials which vary from site to site in a random fashion and the calculation of physical quantities averaged over ensembles of such potentials using the coherent potential approximation (CPA). This facilitates applications of the SIC to alloys and pseudoalloys which could describe disordered local moment systems, as well as intermediate valences. As a demonstration of the method, we study the well-known α-γ phase transition in Ce, where we also explain how SIC operates in terms of multiple scattering theory.

Influence of atomic relaxation on the magnetic properties of Mn/Ni(001) system

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The Mn bulk ground state being essentially of non-ferromagnetic type, a spin flop towards ferromagnetism can be induced by strong 3d ferromagnets (Fe, Co, Ni) [1, 2]. We discuss the

geometric optimization and the onset of ferromagnetism in Mn/Ni(001) system. Spin-polarized (with collinear magnetism) calculations within the density functional approach of *Kohn and Sham* and beyond local density approximation are performed by the pseudopotential code PWscf. This calculations are supported by the recent experimental works [3, 4, 5]. The results obtained showing evidence of NiMn surface alloy formation, a contraction of the Ni atomic positions in the overlayer after relaxation in the cases of Ni(001) clean surface and NiMn alloy on Ni(001) and, an outwards buckling of Mn atoms in the cases of Mn metallic and NiMn alloy on Ni(001).

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Determination of lattice site occupation and oxidation state of Fe and Mn ions in doped $LiNbO_3$ and investigation of structural changes of $Ni_{50}Mn_{30}Ga_{20}$ freestanding films in dependence on the temperature of RTA (Rapid Thermal Annealing) by means of XAS (X-ray Absorption Spectroscopy)

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Physikalisches Institut der Universität Bonn (AG Modrow/Hormes), Nuallee 12, 53115 Bonn, Germany

In the present work experimental XANES (X-ray Absorption Near Edge Structure) spectra of both Mn and Fe (EQ70 and EQ729 sample) in doped $LiNbO_3$, at Mn and Fe K-edge respectively, are analyzed and compared to the calculated using FEFF8 code[1] spectra. In FEFF8 code calculations the FMS (Full Multiple Scattering) approach within the cluster of atoms (within the R=6.35 $\AA$ around absorbing atom) constructed according to the crystal structure data of $LiNbO_3$ (where Mn (Fe) is assumed to be either on Li or Nb site in $LiNbO_3$ matrix) is applied. From analysis of comparison between experimental and calculated with the use of FEFF8 code XANES and PDOS (P Density of states) spectra, the conclusion about lattice site occupation of both Mn and Fe in $LiNbO_3$ matrix is made. The oxidation states of Fe and Mn ions in doped $LiNbO_3$ are determined comparing their corresponding main absorption edge positions at their Fe and Mn K-edge experimental XANES spectra to the appropriate reference spectra.

XANES qualitative analysis results along with FEFF8 calculations and first coordination shell EXAFS (Extended X-ray Absorption Fine Structure) fit at Mn K-edge are also presented in this work for $Ni_{50}Mn_{30}Ga_{20}$ films, as-deposited and annealed at t=200 ^{o}C, 400 ^{o}C, 600 ^{o}C, and 650 ^{o}C. From analysis of experimental XANES and calculated FEFF8 spectra and Modified FT of freestanding $Ni_{50}Mn_{30}Ga_{20}$ films, the dependence of structural disorder of the samples on annealing temperature and existence of different phases of films are obtained. The dependence of structural disorder on annealing temperature is confirmed by first coordination shell Mn-Ni EXAFS fit results.

[1] A. L. Ankudinov, B. Ravel, J. J. Rehr, S. D. Conradson, Phys. Rev. B **55**, 7565 (1998).

Electronic Structure Calculations with Short Range Order

D. Rowlands

University of Bristol—3.56a H.H.Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, UK

For many years the Korringa-Kohn-Rostoker coherent-potential approximation (KKR-CPA) has been widely used to describe the electronic structure of disordered systems based upon a first-principles description of the crystal potential. However, as a single-site theory the KKR-CPA is unable to account for important environmental effects such as short-range order (SRO) in alloys and spin fluctuations in magnets, amongst others. Using the recently devised KKR-NLCPA (where NL stands for nonlocal), we show how to remedy this by presenting explicit calculations for the effects of SRO on the electronic structure of the bcc $Cu_{50}Zn_{50}$ solid solution.

Computing conductances of tunnel junctions by the Korringa-Kokn-Rostoker method : Formulation and test of a Green function approach.

J. Henk, A. Ernst, K.K. Saha and P. Bruno

Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale)

An approach to computing conductances of tunnel junctions within the framework of the Landauer-Büttiker theory for the electronic transport is introduced and formulated for the Korringa-Kohn-Rostoker (KKR) method for electronic-structure calculations. After a general introduction to the idea behind the approach, tests and comparisons with other methods, namely a 'transmission of Bloch-waves' approach and an approach based on the Kubo-Greenwood formula for the conductivity tensor, reveal a high accuracy and robustness of the proposed method, thus proving its suitability for state-of-the-art computations of spin-dependent ballistic transport. Based on Green functions, it is flexible and can easily be implemented in present KKR computer codes.

Magnetic tunnel junctions with Heusler alloy electrode: Interface structure and magnetism explored by soft X-rays

J. Schmalhorst, A. Hütten and G. Reiss

University of Bielefeld, Department of Physics, Nano Device Group, P.O. Box 100131, 33501 Bielefeld, Germany

The implementation of half-metallic materials like full Heusler alloys for spintronic applications, e.g., as electrode in magnetic tunnel junctions, is of highest technological relevance. The major challenge is the preparation of preferably defect free interfaces.

We fabricate Co_2MnSi / AlO_x / Co-Fe MTJs with more than 100% tunneling magnetoresistance (TMR) at low temperature and low bias voltage. However, the TMR bias voltage and temperature dependence is considerably stronger than usually found for optimized MTJs with 3d-alloy electrodes. For explaining this conclusively, knowledge of the structural and magnetic properties of the Co_2MnSi / AlO_x interface is of vital importance. In this talk investigations of the Co_2MnSi / AlO_x interface and the Co_2MnSi bulk material by X-ray absorption spectroscopy will be presented and discussed with respect to the temperature dependent transport properties of the junctions.

The authors gratefully acknowledge the opportunity to perform soft X-ray absorption spectroscopy at the Advanced Light Source, Berkeley, USA and at the BESSY mbH, Berlin, Germany.

Free clusters

O. Šipr

Institute of Physics AS CR—Cukrovarnicka 10, Praha 6, Czech Republic

Clusters comprising few tens or hundreds of atoms form an interesting class of materials, because they form a bridge between atoms and molecules on the one hand and solids on the other hand and yet their properties cannot be described by a simple interpolation between the two extremes. Magnetic properties of transition metal clusters, in particular, attracted a lot of attention recently - both due to fundamental reasons and due to potential applications in magnetic recording technology. As clusters contain a large portion of surface atoms, it is interesting to study the relation between the electronic and magnetic properties of atoms which are close to a cluster surface and of atoms which are close to a planar surface of a crystal. A frequently used tool for studying magnetism in complex systems is x-ray magnetic circular dichroism (XMCD), defined as the difference between the absorption rate for left- and right-circularly polarized x-rays in magnetic targets.

The talk will thus focus on theoretical investigations of electronic, magnetic and spectroscopic properties of free Fe clusters of 9 to 89 atoms with bcc geometry and bulk interatomic distances and on comparing their properties with properties of bulk Fe and of bcc-Fe crystal surfaces.

The theoretical framework is based on an ab-initio fully-relativistic spin-polarized real-space multiple-scattering technique, as implemented in the SPRKKR code.

X-ray absorption spectroscopy analysis of small nanoclusters

A.V.Soldatov[1,4], G. E.Yalovega[1], V. Mazalova[1], S. Adam[2], A. Lobo[2] and T.Möller[3]

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[2] *HASYLAB at DESY, Hamburg, Germany*
[3] *Department of Physics, TU Berlin, 10623 Berlin, Germany*
[4] *LNF INFN Frascati Italy*

Free and supported clusters of atoms are the novel physical objects which probably can make a bridge from atomic to solid state physics. Therefore the study of their structure and electronic subsystem in a function of cluster size is of great importance. The status of modern research shows XANES spectroscopy to be a useful tool for the investigation of both local structure and electronic subsystem of free clusters. X-ray absorption spectra of clusters with different type of chemical bonding covering the whole size range from several atoms to the solid are reported. The clusters have been generated using 'pick-up' method and their XANES spectra have been measured by both TEY and Auger YIELD techniques at BW3 beamline of HASYLAB at DESY. The x-ray absorption fine structure is shown to be sensitive to the size of cluster. For theoretical analysis of the experimental spectra a modern, self consistent full multiple-scattering method has been applied. In the framework of this approach dependence of the XANES vs. the cluster size has been analysed. In order to study the sensitivity of XANES on cluster symmetry, theoretical simulations have been performed for different structural models.
Part of the research is supported by the grants fo the President of Russian Federation (MK-2048.2004.2) and UNIROS, Russia (UR.01.01.271).

X-ray absorption spectroscopy of SiC

M. Tallarida and D. Schmeisser

Brandeburgische Technische Universität, Konrad Wachsmann Allee 17, 03046 Cottbus

We have measured X-ray absorption spectra (XAS) of 3C- and 4H- SiC at the Si-$L_{2,3}$ and C-K edges. For the two polytypes the near edge spectra are very different in shape. We have compared our spectra with total and partial density of states calculations, addressing the various XAS features to Si- and C-derived states. By considering the different crystal structure symmetry of the two polytypes, we can put in evidence the influence of electronic band symmetry in the absorption cross sections of both edges.

Multiple Scattering Theory: KKR and KKR-CPA
I. Ordered Systems
II. Disordered Systems

W.M. Temmerman and Z. Szotek

Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK

In these talks we briefly overview the multiple scattering theory and elaborate on the KKR and KKR-CPA methods that are based on this theory. In the first part we derive the single scatterer and multiple scattering quantities, leading to the single particle Green's function from which a number of observables can be calculated. Screened structure constants and impurity Green's functions are introduced and applications to surfaces and interfaces are also briefly discused. In the second part we concentrate on disordered systems and discuss the KKR-CPA band structure method in some detail. We introduce the configurationally averaged Green's function, density of states, integrated density of states, and spectral functions. The power of the method is demonstrated by showing that one can not only study real substitutional alloys, composed of different elements, but can utilize the alloy analogy to describe properties of pseudo alloys, comprising different phases of a system, as for example localized (γ) and delocalized (α) phases of Ce. The calculated finite temperature phase diagram of Ce α to γ phase transition is discussed to illustrate the great potential of this methodology.

Ab initio simulation of deformation of nanostructure and its relation to electronic properties

Y. Umeno

Institut fuer Zuverlaessigkeit von Bauteilen und Systemen (IZBS), Universitaet Karlsruhe (TH), Germany

(Department of Engineering Physics and Mechanics, Kyoto University, Japan)

Nanostructures have been attracting attention because of their prominent properties, and their applications for novel devices with advanced functions have been attempted. Since such nanostructured materials are subject to high strain conditions it is important to clarify the mechanical properties and its relation to electronic structure. We have conducted ab initio simulations to elucidate the mechanical and electronic properties of materials placing our focus on the behavior of materials under high strain condition. Single crystal such as silicon and silicon carbide under ideal shear is investigated to find the relation between deformation and electronic structure. Tensile simulation of silicon thin film is performed to manifest the effect of surface structure on the mechanical properties and the electronic structure. The mechanical and electronic properties of carbon nanotubes under large deformation are also introduced. Investigation of structure and properties of perovskite thin films and ferromagnetic materials will be our future project.

A new X-ray Spectrometer with large Focusing Crystal Analyzer

E. Welter[1], P. Machek[2], G. Dräger[3], U. Brüggmann[1] and M. Fröba[2]

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[3] *Fachbereich Physik der Martin-Luther-Universität Halle-Wittenberg, Germany*

A new focusing spectrometer in Johann geometry that was build and permanently installed at the wiggler beamlime W1 at the Hamburger Synchrotron Strahlungslabor (HASYLAB) am Deutschen Elektronen Synchrotron (DESY) is described. It is now available for user operation. The usable energy range of the spectrometer which is installed inside a vacuum tank is 2.1 keV - 25 keV. Currently it is however limited by the source to 4.5 keV - 10.5 keV. The design of the spectrometer is optimised for the usage of a large source spot size at the DORIS storage ring as well as for simple operation and robustness under the conditions of user operation. Nevertheless, in the future, an undulator at a PETRA III beamline would be the ideal source to enlarge the number of possible applications. The spectrometer uses spherically and cylindrically bent crystals with typical bending radii of 100 cm (spherical) and 70 cm (cylindrical). The performance of the spectrometer is demonstrated by three bench mark experiments, Resonant Inelastic X-ray Scattering (RIXS), X-ray Absorption Fluorescence Spectroscopy (XAFS) in samples with complicated matrices and the determination of the chemical shift of Kβ emission lines of Cr in different valence states.

XAS of light 3d elements: a benchmark for *ab initio* calculations

H. Wende[1], A. Scherz[1], C. Sorg[1], N. Ponpandian[1], M. Bernien[1], K. Baberschke[1], J. Minár[2], H. Ebert[2]

[1] *Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem, Germany*
[2] *Institut für Physikalische Chemie, Universität München, Butenandtstraße 5-13, D-81377 München, Germany*

The element- and shell-specific XMCD technique provides a unique tool for the investigation of the magnetism of ultrathin films and nanostructures. Detailed fine structures in the L-edge XMCD are resolved at the new generation synchrotron sources. They allow for the study of the induced magnetism of light 3d elements like Ti, V and Cr at the interface to ferromagnetic layers [1-3]. However, it turns out that for these elements the strong electron-hole interaction leads to a shift of the spectral weights from the L3 to the L2 edge and thereby to the breakdown of the standard analysis (sum rules). Therefore, *ab initio* calculations were performed with the Munich SPR-KKR package to determine the magnetic ground state properties of these systems and the corresponding X-ray absorption spectra. Furthermore, a double-pole approximation within the time-dependent DFT will be presented, which allows for an experimental assessment of the exchange-correlation kernel. The experimentally determined correlation energies can be used to

test advanced exchange kernels in the future. This work is supported by BMBF (05 KS4 KEB/5).

[1] H. Wende, Rep. Prog. Phys. **67** 2105 (2004).

[2] A. Scherz, H. Wende, K. Baberschke, Appl. Phys. A **78** 843 (2004).

[3] A. Scherz, H. Wende, K. Baberschke, J. Minár, D. Benea, H. Ebert, Phys. Rev. B **66** 184401-1 (2002).

Interface effects observed by magneto-optical Kerr effect of ultrathin transition metal films on palladium substrates

A. Winkelmann, M. Przybylski, M. Nyvlt, Y. Shi, J. Barthel, J. Kirschner

MPI für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We have measured the magneto-optical Kerr effect (MOKE) of ultrathin iron and cobalt films epitaxially grown on palladium substrates of different crystallographic orientations. Anomalous changes in the Kerr rotation observed at low thicknesses of the films are attributed to the influence of the interface between the ultrathin film and the substrate. In particular, sign reversals of the Kerr signal are observed. Due to the complexity of the magneto-optical response, no direct conclusions can be drawn about the magnetic moments at the interface. However, it could be possible to attribute the measured effects to influences from the electronic and spin structure of the interface. Theoretical calculations of MOKE for different compositions and magnetic configurations of the Co/Pd and Fe/Pd interfaces would be helpful in this case.

Electronic and magnetic properties of the surfaces and interfaces of hole doped manganites from model and first principles calculations

H. Zenia[1,2], G. A. Gehring[1] and W. M. Temmerman[2]

[1] *Department of Physics and Astronomy, University of Sheffield*
[2] *Daresbury Laboratory, Daresbury*

The electronic and magnetic properties of hole-doped manganite surfaces are investigated in a model and a Self-Interaction Corrected (SIC-LSDA) calculations. The model incorporates the kinetic energy of the e_g electrons, their coupling through Hund's rule to the core-like t_{2g} spin and the superexchange interaction between the latter. A shift is added to the onsite energy at the surface in order to mimic the effects of the changes with respect to the cubic symmertry in the bulk. We looked at negative values of the shift added to one orbital or both with respect to the bulk levels. We found that the most favourable scenario is when a small shift is added to the $3z^2$-r^2. The stability of the ferromagnetic (FM) coupling between surface and bulk is enhanced as a result. But a larger shift would deplete the other orbital and thus would disfavour in-plane FM coupling at the surface which would be detrimental to the tunnelling magnetoresistance (TMR)

of manganite-based junctions. In the SIC-LSDA calculation we found that the subsurface Mn ion localises an extra e_g electron whereas when at the surface only the t_{2g} orbits are localised. We have also studied $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ within SIC-LSDA to look at the interfaces. Important changes are found to occur at the interface but given that we used only one unit cell for $SrTiO_3$ this becomes metallic. We are looking at bigger cells and also different interfaces, ie La-Ti and Mn-Sr.

SIC-LSD Description of Spintronics Materials

Z. Szotek[1], W.M. Temmerman[1], T. Schulthess[2],
L. Petit[2], G.M. Stocks[2], A. Svane[3], P. Strange[4],
and H. Winter[5]

[1] *Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK*
[2] *Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA*
[3] *Institute of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark*
[4] *Department of Physics, Keele University, UK*
[5] *IFP, Forschungszentrum Karlsruhe GmbH, Postfach 3640, D-76021 Karlsruhe, Germany*

We discuss an application of the self-interaction corrected local spin density approximation (SIC-LSD) to half-metallic transition metal oxides, and among them double perovskites and magnetite (Fe_3O_4), and diluted magnetic semiconductors such as Mn-doped Ga-group V compounds and ZnO. In addition we explore also spinel ferromagnetic insulators for exploiting in spin filtering heterostructures. Also, Eu chalcogenides and pnictides, as well as rare earth sulphides, are scrutinised for possible technological applications. We concentrate on the electronic and magnetic properties of all the compounds and in magnetite, in addition, issues of charge order are also thoroughly investigated.

3 General Workshop/Conference Announcements

3.1 RSC Faraday Discussion Meeting: ATOMIC TRANSPORT & DEFECT PHENOMENA IN SOLIDS

Call for Papers

10-12, July 2006 (University of Surrey, Guildford, UK)

http://www.rsc.org/ConferencesAndEvents/RSCConferences/FD134/index.asp

Details on the meeting can be found on the website above. Invited speakers listed is given below.

Confirmed invited speakers:

Professor Peter Bruce, University of St Andrews, UK
Professor Clare Grey, SUNY Stony Brook, USA
Professor Sossina Haile, Caltech, USA
Professor Paul Heitjans, Hannover University, Germany
Professor John Kilner, Imperial College, UK
Professor Joachim Maier, Max-Planck-Institut für Festkörperforschung, Germany
Professor Linda Nazar, University of Waterloo, Canada
Professor Dieter Wolf, Argonne National Laboratory, USA
Professor Masatomo Yashima, Tokyo Institute of Technology, Japan
Professor Maylise Nastar, CEA Saclay, France

3.2 CNF Fall Workshop: Modeling the Nanoscale World

Cornell Nanoscale Science and Technology Facility, Ithaca, NY

October 10th-12th, 2005

Organized by the NNIN/C

(http://www.nnin.org/nnin_compsim.html)

Sponsored by the National Science Foundation

Workshop Coordinator: Derek Stewart (stewart@cnf.cornell.edu)

http://www.cnf.cornell.edu/cnf_2005fallworkshop.html

The nanoscale regime provides an important arena where scientific disciplines converge to study systems that can have tremendous fundamental and commercial impact. Computational approaches provide a crucial window into the nanoscale world. These codes help explain nanoscale phenomena and guide future studies. However, in order to successfully use these computational techniques with experimental tools, researchers must learn about the principles and areas of application associated with each code.

This workshop will provide introductions on several computational approaches that are essential for nano-materials, nano-chemistry, and nano-photonics. Morning lectures on the theory behind approaches will be followed by *hands-on* afternoon sessions on each code. In some cases, the participants will be able to learn directly from the code's creator. Graduate students and young researchers with theory or experimental backgrounds are encouraged to attend. More seasoned members of the field are also encouraged to come and share their knowledge.

Tutorials will be provided on codes such as Abinit, LM Suite, Layered KKR, NWChem, CPMD, MIT Photonic Bands, and FDTD approaches.

Poster Abstract Deadline: August 26th, 2005
Registration deadline: September 9, 2005
Seating is limited to 30-40 participants. Please register early!

3.3 International Symposium on Spin- and Charge-Correlations in Molecule-based Materials

Koenigstein (near Frankfurt a.M.), Germany
October 17-19 2005

For more information please visit the website

http://www.itp.uni-frankfurt.de/forschergruppe412/symposium/

Maria-Roser Valenti
Institut für Theoretische Physik,
Universität Frankfurt,
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e-mail: valenti@itp.uni-frankfurt.de

3.4 DFTEM 2006 Conference

First Announcement

DFTEM 2006

"bringing together two communities: DFT + TEM"

21 - 23 April, 2006 – Vienna, Austria

`http://www.physics.at/dftem2006`

The Conference: April 21-23, 2006

This three-day conference will focus on Density Functional Theory (DFT) and Transmission Electron Microscopy (TEM) with the intention of bringing together these two communities. The conference is dedicated to Karlheinz Schwarz (DFT) and Bernard Jouffrey (TEM) on the occasion of their respective birthdays, which we will celebrate at the conference dinner. The conference will follow two days of separate workshops for the two fields.

The Workshops: April 19 & 20, 2006

12th WIEN2k Workshop

This WIEN workshop deals with density functional (DFT) calculations of solids using the (full-potential) Augmented Plane Wave plus Local Orbitals (APW+lo) method as embodied in the WIEN2k code (`http://www.wien2k.at`) and related topics.

2nd CHIRALTEM Workshop

The CHIRALTEM project (`http://www.chiraltem.physics.at`) is one of the ten STREPs (Specific Targeted Research Projects) within the NEST (New and Emerging Science and Technology) support actions of the European Community.

Fees + Registration

Workshops:	EUR 100
Conference:	EUR 250
Combi-Pack:	EUR 300 (available until December 24, 2005)
Student-Combi:	EUR 200 (when registering until December 24, 2005; proof of the student status is required)

The fee for the conference includes coffee breaks, conference dinner and conference book.
For the WIEN2k workshop the number of participants is limited!
Preliminary registration, registration, abstract submission and more information is available at `http://www.physics.at/dftem2006`.

Scientific Program

The scientific program of the conference will include invited talks, contributed talks and posters. Extended and refereed abstracts will be published. Invited speakers confirmed so far include:

Ole K. Andersen, MPI Stuttgart, Germany	**Lucia Reining**, École Polytechnique, France
Peter E. Blöchl, Clausthal University of Technology, Germany	**Matthias Scheffler**, FHI Berlin, Germany
Gianluigi Botton, McMaster University, Hamilton, Canada	**Virginie Serin**, CENES, France
Frank de Groot, Universiteit Utrecht, Netherlands	**Eric L. Shirley**, NIST, USA
Börje Johansson, Uppsala University, Sweden	**David Singh**, Oak Ridge NL, USA
Klaus Leifer, Uppsala University, Sweden	**Susanne Stemmer**, UC Santa Barbara, California, USA
Georg Madsen, University of Aarhus, Denmark	**Isao Tanaka**, Kyoto University, Japan
Manu Perez-Mato, Univ. de Pais Vasco, Bilbao, Spain	**Samuel B. Trickey**, University of Florida, Gainesville, Florida, USA
John J. Rehr, University of Washington, Seattle, USA	

The programs for the workshops will be communicated at a later stage.

Organizing Committee

* Claudia Ambrosch-Draxl, Uni Graz, Austria * Peter Blaha, TU Wien, Austria * Clemens Först, MIT, USA * Cécile Hébert, TU Wien, Austria * Kerstin Hummer, Uni Wien, Austria * Kevin Jorissen, Universiteit Antwerpen, Belgium; U. of Washington, USA and IAST Austria

* Dieter Kvasnicka, TU Wien, Austria * Joachim Luitz, IAST Austria * Pavel Novak, Czech Academy of Sciences, Czech Republic * Peter Schattschneider, TU Wien, Austria * Jorge O. Sofo, Pennsylvania State University, USA * Michael Stöger, TU Wien, Austria * Marc Willinger, FHI Berlin, Germany

This conference is organized by the association "Physicae et chimicae solidorum amici" in co-operation with the Institute of Material Chemistry and the Institute of Solid State Physics of the Vienna University of Technology (TU Wien), Austria.

Contact

DFTEM 2006
c/o IAST Austria
Wohlmuthgasse 18
A-3003 Gablitz/AUSTRIA

dftem@physics.at
www.physics.at/dftem2006

3.5 NIC Winter School 2006

"Computational Nanoscience: Do it Yourself"

Forschungszentrum Jülich, Germany

14-22 February, 2006

http://www.fz-juelich.de/conference/wscn

For details please check the above web page.

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Phone: +49 2461 61 6585

Fax: +49 2461 61 6656
URL: http://www.fz-juelich.de/zam

3.6 Symposium on "Explicit density functional of the kinetic energy in computer simulations at atomistic level"

"International Conference of Computational Methods in Sciences and Engineering (ICCMSE2005)"

Loutraki, Korinthos, Greece

21-26 October, 2005

`http://www.uop.gr/~iccmse/`

The original deadline for submitting extended abstracts for the above symposium has been extended until August 5, 2005. Anybody interested is invited to submit a paper. For more details see the symposium web-page:

`http://lcta.unige.ch/~tomek/dft2005_symposium.html`

or contact directly Tomasz.Wesolowski@chiphy.unige.ch.

3.7 Symposium on "Semiconductor nanocrystals and nanoclusters"

"International Conference of Computational Methods in Sciences and Engineering (ICCMSE2005)"

Loutraki, Korinthos, Greece

21-26 October, 2005

`http://www.uop.gr/~iccmse/`

The deadline for submitting papers and abstracts for the symposium on:

"Semiconductor nanocrystals and nanoclusters"

of the "International Conference of Computational Methods in Sciences and Engineering (ICCMSE2005)" in Loutraki, Korinthos, Greece, on 21-26 October 2005, has been extended till August 5, 2005.

The extended abstracts (up to four A4 pages) submitted for all symposia at this conference will be published in a special volume of the "Lecture Series on Computer and Computational Sciences". The volume will be available at the time of the conference. In addition, several of the submitted papers will be considered further for publication in other regular journals. Papers (oral presentations or posters) concerning topics of relevance to the main subject of the session in the fields of chemistry, physics, computer modelling, nanoscience etc. are most welcome. You can send your contribution directly to me at zdetsis@upatras.gr or directly to the conference organizers

I would like to bring to your attention the fact that this year's edition of ICCMSE is an interdisciplinary conference with only a few plenary talks and a large number of specialized parallel sessions (symposia). The list of other symposia can be found at the web-site :

`http://www.uop.gr/~iccmse`.

Sincerely,

A.D. Zdetsis

3.8 International Workshop on "Ab-initio Description of Iron and Steel (ADIS-2006): Status and future challenges"

February 19-24, 2006

Ringberg Castle (Tegernsee, Germany)

http://adis-2006.mpie.de

In February 2006 an international workshop on recent developments of an "Ab-initio description of iron and steel" will be held at Ringberg castle (Germany). The focus of the meeting will be on the combination of ab-initio approaches with various thermodynamic and kinetic concepts to model finite-temperature properties/processes and phase transitions of realistic materials such as metal alloys.

Key experts in both fields have been invited to give tutorial-like lectures on recent methodological advances and future applicational challenges. All participants have the opportunity to present their results in poster sessions. A selected number of 30-minute oral contributions will also be possible.

To provide ample time for discussion and exchange the workshop is restricted to 40 participants (incl. invited speakers). In order to register for the workshop, please send an e-mail to adis2006@mpie.de. The selection will be on a first come first served basis. The final

deadline of registration is December 1, 2005.

The conference fee of 700 EURO covers full-board accommodation from 19th of February (dinner) until 24th of February (breakfast) 2006, the abstract booklet, social events and the conference dinner. The workshop is organized by the Computational Materials Design department (http://www.sfhingx.de/cm/), recently established at the Max-Planck-Institute for iron research in Duesseldorf (Germany).

4 General Job Announcements

POSTDOCTORAL POSITION IN CONDENSED MATTER THEORY/MODELING

UNIVERSITY OF SOUTH FLORIDA

Applications are invited for postdoctoral position in theoretical & computational condensed matter & materials physics. The work will involve research on first-principles theory of tunneling in condensed matter and molecular systems and atomistic modeling of nanostructured materials.

The successful candidate must have a Ph.D. in theoretical or computational physics, chemistry, materials science or closely related fields. He/she must have demonstrated the ability to develop new theoretical methods and implement these methods in computer programs. The candidate should have an experience with electronic structure methods including density functional theory, tight-binding and other atomistic modeling techniques.

The appointment is initially for one year, with the possibility of renewal. The position is available immediately. Applicants should send a letter of application, curriculum vitae, a statement of research experience and interests, list of publications, and list of 3 references to Prof. Ivan Oleynik at oleynik@shell.cas.usf.edu.

Ph.D. studentships are also available.

POSTDOCTORAL FELLOWSHIP

Uppsala University, Sweden

A postdoctoral position will be available at Uppsala University, starting from October 2005, for a period of up to 3 years.

The research will be on electronic properties of biomaterials, using ab initio DFT-based calculations. Also, theoretical modelling of various functional properties of complex biological materials will be performed, based on the performed ab initio calculations, aiming at describing and predicting medical functionality. The research will be conducted together with experimental groups in Europe within a multidisciplinary EU-funded research collaboration.

The candidate is expected to have a strong background in computational chemistry or computational physics. Experience with large scale ab initio calculations is desirable, as is also the ability to collaborate in a multidisciplinary environment.

A strong research environment in computational material science exist at the Physics Department of Uppsala University, which will provide an excellent scientific working place for the postdoc.

To apply, please send a CV, list of publications, and names of two reference persons, to Peter Oppeneer, at the address given below. Applications are expected to be considered until the end of August.

Peter Oppeneer,
Assoc. Prof., Dept. of Physics,
Uppsala University, Box 530
S-751 21 Uppsala, Sweden
peter.oppeneer@fysik.uu.se

POSTDOCTORAL FELLOWSHIP in COMPUTATIONAL CHEMISTRY

at CEA Laboratories, SACLAY, FRANCE

Applications are being sought for a postdoctoral position in my group at the "Commissariat a l'enegie Atomique" (the French atomic energy commission or CEA), in Saclay (Paris region). The position is for one year and can be extended for a second year by mutual agreement. The starting date is flexible, but the postdoctoral fellow need begin before the end of 2005.

An appropriate candidate should have a Ph.D. in Physical Chemistry, Chemical Physics, Physics, Biophysics, or related fields. Also, the candidate should have experience with ab initio DFT calculations on complex molecular systems. Knowledge of molecular dynamics simulation techniques would be an advantage.

The postdoctoral fellow will study the mechanism of oxygen production in photosystem II by computational means. In particular, we plan to investigate the electronic states and conformational properties of oxygen evolving center - a cubane-like Mn3CaO4 aggregate connected to another Mn ion through an oxygen bridge - the structure of which has been recently obtained for the cyanobacterium Thermosynechoccus elongates at atomic resolution.

To apply, please send an email describing the candidate research interests and achievements together with a complete CV, including the names of at least two referees, to Dr. Massimo MARCHI (Massimo.Marchi@cea.fr).

Because of internal rules of CEA, at the date of hiring not more than three (3) years must have passed from the PhD of the successful candidate. CEA provides a competitive salary and a complete health insurance and retirement package for postdocs.

Dr. Massimo MARCHI
Commissariat a l'Energie Atomique
DSV-DBJC-SBFM
Centre d'Etudes de Saclay
Gif sur Yvette, Paris, FRANCE

Post-Doctoral Research Associate

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

Applications are invited for a Research Associate position jointly funded by the Engineering and Physical Sciences Research Council and the UK Ministry of Defence. Funding is available to support the position for up to three years.

The aim of the research project is to use atomistic computer modelling based on first-principles quantum mechanics to investigate the properties of metals under extreme conditions. The work will employ theoretical methods developed at UCL in the Physics and Astronomy and the Earth Sciences Departments for studying the properties of iron in the Earth's core. The work will be performed at UCL under the supervision of Professor Mike Gillan, Professor David Price, and Dr. Dario Alfe.

Candidates must have, or expect to obtain, a Ph.D. in a relevant physical science. A thorough practical knowledge of quantum mechanics and condensed matter physics is essential, as is experience with computational methods, preferably involving high-performance computing. A good knowledge of statistical mechanics will be an advantage.

The appointment will be made on the RA1A scale. The starting salary will depend on age and experience, but will be not less than 21,640 per annum plus 2330 London Allowance.

Informal enquiries to Professor Mike Gillan (m.gillan@ucl.ac.uk) are encouraged. Such enquiries must include a CV and the names and e-mail addresses of three academic referees. Formal applications, accompanied by a CV, should be made by downloading an application form from:

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

Further details can be obtained from:

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

Closing date: 23 September 2005

UCL Taking Action for Equality

POST-DOCTORAL POSITIONS in CONDENSED MATTER THEORY

Department of Physics, University of Missouri, USA

Applications are invited for two post-doctoral positions in theoretical and computational condensed matter physics and materials theory. The work will involve research in the area of materials theory including semiconductor spintronics materials such as GaAs(Mn) and correlated oxide systems such as perovskite oxides. One of the positions will involve methods development and calculations using density-functional theory, while the second one could be in the more general area of correlated electron solids using analytical tools. For the first position, experience with electronic structure methods including density functional theory is highly desirable. The initial appointment for both positions will be for one year and may be renewed for up to two more years subject to availability of funding. We encourage applications from creative individuals with out-of-the-box research thinking and with a solid background in condensed matter theory. My group consists of typically two graduate students, two post-docs, and two to three highly interactive summer visitors. The group's expertise is in the density-functional calculations using mostly the LMTO method, but a variety of projects in condensed matter physics is also undertaken which do not require expertise in the DFT methods.

Interested candidates should send a letter of interest, a curriculum vita, two to three papers describing previous research, and arrange to have three letters of reference sent electronically to: satpathys@missouri.edu (pdf files work best for me) or by regular mail to: Prof. S. Satpathy, Department of Physics, University of Missouri, Columbia, MO 65211, USA. Full consideration of applications will begin July 15, 2005 and will continue until the positions are filled.

Postdoctoral and Ph.D. Positions

Computational Materials Science

Institut für Materialphysik, Universität Wien
http://cms.mpi.univie.ac.at

A postdoctoral and a Ph.D. position are available, to begin in July 2005, associated with Prof. Georg Kresse, Computational Materials Science Group at the Institute for Materials Science, University of Vienna. The group has developed and maintains the Vienna ab initio package (**VASP**), which is used worldwide by 500 academic and industrial groups. An **outstanding environment** for acquiring first hand knowledge on density functional computations and program development is offered with special graduate courses for PhD students and a total of 40 scientists and PhD's working in this field.

The research will be performed in the field of DFT within the framework of a national Joint Research Program (JRP-S9008-N02), which comprises both experimental and theoretical groups. The candidates should have the ability to communicate with all the involved groups. The research program aims on the investigation and development of new nano-structured surfaces based on metallic or oxidic supports and ultra-thin layers, involving also correlated systems which need treatments beyond the local density approximation. The candidates are required to have appropriate education in solid state physics, surface science, and experience in applying electronic structure total energy codes. Programming skills (FORTRAN 95, MPI) would be very welcome for implementing tools, e.g. for spectroscopy.

Interested applicants should send (1) a CV including a publication list, (2) one or two reprints representative of previous research, and (3) two confidential letters of recommendation to:

Ao. Univ.-Prof. Georg Kresse
Institut für Materialphysik
Universität Wien
Sensengasse 8/12
A-1090 Wien, AUSTRIA

or

Georg.Kresse@univie.ac.at

Please note: When sent by email, the application should include the CV and reprints as pdf files as well as a short cover letter in the email body. The letters of recommendation should be sent directly by the referees.
Consideration of candidates will begin immediately and will continue until the positions are filled.

EPSRC Studentship

High End Computing for the Characterisation of Structure and Reactivity of Complex Oxide Catalysts

Royal Institution of Great Britain
and
Computational Chemistry Group, CCLRC Daresbury Laboratory, UK

An EPSRC Studentship is available from October 2005 to work with the Royal Institution of Great Britain and the Computational Chemistry Group, CCLRC Daresbury Laboratory into the modelling of complex catalytic systems using high-performance computing.

The four year studentship is expected to lead to the award of an MSc in High-End Computing (awarded by the University of Edinburgh) and a PhD (awarded by University College, London).

The project will use sophisticated molecular modelling techniques incorporating quantum mechanical methods such as Density Functional Theory. We plan to study a variety of materials, focussing on complex catalysts containing finely dispersed transition metals carried on a variety of mineral supports. The methods we are developing allow the study of possible reaction mechanisms and the determination of properties of adsorbed species for comparison with experiment.

The first year of the project will be spent at CCLRC's Daresbury Laboratory in Cheshire, learning the technical details of the software and methodology and optimising its performance on the UK's leading national computing facilities. The remainder of the project will be based at the Royal Institution in London. The taught MSc is expected to involve two visits to Edinburgh (each of 2 months duration) to attend courses on parallel processing and computational chemistry.

Candidates for the studentship will be expected to hold, or be about to receive, a good Honours or Masters degree in a relevant discipline and should demonstrate a strong interest in computational chemistry. Candidates should also have or expect to acquire a good working knowledge of the principles of chemistry or physics and good computational modelling skills.

The Studentship includes financial support for fees at the University College, London and the University of Edinburgh, travel costs for the stays in Edinburgh, and a stipend, subject to the usual eligibility requirements. For further details contact Prof Catlow or Dr Sherwood:

Email:	richard@ri.ac.uk	p.sherwood@dl.ac.uk
Tel:	020 7670 2901	01925-603553
Fax:	020 7670 2958	01925-603634

Applications, including a CV, should be sent as soon as possible to Professor Catlow.

Post-Doctotal Postion at CEA/Direction des Applications Militaires

Bruyeres-Le-Chatel, France

MOLECULAR DYNAMICS STUDY OF WARM DENSE PLASMA OF LANTHANIDE

Warm dense plasma physics is the transition regime between cold materials and hot dense plasma (ionised gas). Understanding the warm dense regime is important for the study of materials in extreme conditions (high pressure and high temperature) as it is encountered in astrophysics or in laser-matter interactions. The goal of this post doctoral stage is to compute the equation of states and the electronic transport properties using ab initio methods for a lanthanide in the warm dense regime (solid ionic density divided by ten and temperature from 10000K to 30000K). The theoretical results will be compared to experimental data obtained in the laboratory at the same time.

The candidat must have a Ph.D in computational physics, chemistry and he/she must have a significant experience with first principle electronic structure calculation, in particular density functional theory methods, and pseudo-potential approach.

The position is available for the beginning of 2006 and the contrat is for one year, renewable for a second year upon mutual agreement. To postulate, the candidat should send a curriculum vitae to Dr. Vanina Recoules at vanina.recoules@cea.fr.

Note that in conformity with the CEA's policy, this position is open to recent Ph.D.'s, no more than two or three years after graduation. Individuals who expect to receive their Ph.D. within the next few months are encouraged to apply.

Post-doctoral Research Associate in Condensed Matter Theory

Cavendish Laboratory, Cambridge, U.K.

Grade: NRAS Salary: £19,460 - £29,127 pa

Limit of tenure 31 March 2008

An EPSRC funded post-doctoral position is available for up to 30 months from 1 September 2005 in the Theory of Condensed Matter Group. This post is to work with Dr Chris Pickard on the development and application of a first-principles approach based on pseudopotentials for the calculation of J couplings. The project is a collaboration with the experimental solid-state NMR group of Dr Steven Brown at Warwick. The ideal candidate will have experience of first principles calculation of NMR parameters and NMR experiments, or at least an expertise in one of the foregoing and a desire to learn the other.

Applications together with curriculum vitae, two letters of recommendation and a form PD18 obtainable from

http://www.admin.cam.ac.uk/offices/personnel/forms/pd18

should be sent to Mrs. Tracey Ingham, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, or by email to ti201@cam.ac.uk.

The University offers a range of benefits including attractive pension schemes, family friendly policies, health and welfare provision and staff discounts. The University is committed to equality of opportunity.

The closing date for applications is 5 August.

See

`http://www.tcm.phy.cam.ac.uk/vacancies/further_details.pdf`

for more information.

Marie Curie Host Fellowship for PhD Students

"Ab-initio calculations of many-body effects in electronic spectra"

Laboratoire des Solides Irradies, Ecole Polytechnique, Palaiseau Paris, France

A Marie Curie host fellowship for PhD students is available at the Laboratoire des Solides Irradies, Ecole Polytechnique, Palaiseau (Paris, France), in collaboration with Dr. H.-Ch. Weissker in the group of Dr. Lucia Reining. The fellowship is for 6 months. The research will be inserted in the framework of ongoing collaborations within the EU Network of Excellence NANOQUANTA: Nanoscale Quantum Simulations for Nanostructures and Advanced Materials. The overall topic of the network research is the theory of nanometer-scale structures and the spectroscopic processes that can be used to characterize those structures, their electronic and optical properties, and their growth. These are studied using fundamental theory and state-of the-art ab-initio computer simulations. (Please see also

http://www.cmt.york.ac.uk/nanoquanta/).

In particular, the group in Palaiseau has been working during the last years in the field of one- and two-particle Green's functions calculations (GW, excitons in optical absorption), and time-dependent density-functional theory. These topics should be developed further, concerning both theory and numerics. Computer codes are already available in Palaiseau. Computational facilities include locally several Compaq DS-25 Workstations, and national supercomputer time.

The project includes the ab-initio calculation of quasiparticle energies as well as of the spectral function within different refinements of the GW method and beyond, based on different pseudopotential descriptions of the solid. Silicon will be used as benchmark system, whereas other materials might also be studied.

This work will have two components, one numerical and the other theoretical. In the latter, the applicant will study exchange and correlation effects in the response functions, both using time-dependent density functional theory and Green's-function based methods. The numerical part will consist in contributions to the development of new numerical tools of "theoretical spectroscopy".

The candidate should be working on a thesis subject close to these topics. He/she should have a strong background in theoretical condensed-matter physics including numerics, and should like to perform both analytical and numerical work. As the work will contribute to the nanostructure-related efforts of the NANOQUANTA network, previous experience with nanostructure physics

is desirable in order to carry out the project in view of the final applications.

Candidates must be nationals of an EU Member or Associated State, or have resided in the EU for at least five years immediately prior to their application. They must not undertake their fellowship in the country of their nationality or recent center of activity. At the time of selection the candidate must be 35 years old or less.

The position is intended for the duration of 6 months, starting from October 2005. The deadline for applying for this position is 31/07/2005.

Information on the group can be found at

http://theory.polytechnique.fr.

Contact: Please send your application and brief resume as well as other questions to

hansi.weissker@polytechnique.fr.

Dr. Hans-Christian Weissker
Laboratoire des Solides Irradies
Ecole Polytechnique
F-91128 Palaiseau Cedex
Tel. ++33-1-69 33 36 93
Fax. ++33+1+69 33 30 22
email: hansi.weissker@polytechnique.fr http://www.ifto.uni-jena.de/ hcw/

POSTDOCTORAL RESEARCH ASSOCIATE POSITION IN QUANTUM ELECTROCATALYSIS AT CASE WESTERN RESERVE UNIVERSITY

The research will employ Gaussian molecular and VASP band theory calculations and experience with these or similar techniques is necessary. The position begins in September and will be for one year. Continuation may be possible. The research focuses on modeling fundamental electrode surface reactions and in defining the characteristics of successful electrocatalysts.

Please apply to:

Professor Alfred B. Anderson
Department of Chemistry
Case Western Reserve University
Cleveland OH 44106
Telephone: 216 368 5044
Fax: 216 368 3006
e-mail: aba@po.cwru.edu

Please include your cv with your application including contact data for three or more references, but ask three references to send a recommendation letter.

Electrochemistry spans several departments in addition to Chemistry at Case and activities at the University present opportunities for gaining a broad perspective of the field. Case Western Reserve University is an equal opportunity, affirmative action employer and encourages applications from women and minorities.

Research Associate

"Advanced Atomistic Modelling of Multi-Layer Optical Coatings"

Computational Materials Science Group
Department of Chemistry
Imperial College London, U.K.

An EPSRC sponsored postdoctoral fellowship is available for 3 years in the Department of Chemistry, Imperial College London. You will work within an internationally recognised team of scientists in studies of the composition, structure and electronic structure of functional coatings. Typical optical coatings are nanostructures consisting of several different oxide or metal layers deposited on a glass or polymer substrate. They are used as anti-reflective films on spectacle lenses, UV and infra-red blockers, lighting filters, conductive oxides for flat screen displays and solar control coatings on windows. The design and optimization of coatings requires a basic understanding of the effects of surface and interfacial composition, defects and impurities on mechanical and optical properties. This project will shed light on these fundamental questions through a combination of first principles simulations and empirical modeling.

The project is part of an EPSRC Materials Modelling Consortium involving researchers from 6 universities and 2 industrial partners.

You should have a PhD and a strong research track record in theoretical physics, chemistry or a related discipline. A background in advanced scientific computing and experience of electronic structure theory is also desirable.

The salary will be in the range of £22,116 to £26,652 per annum, depending on qualifications and experience.

Further information can also be found on; http://www.ch.ic.ac.uk/harrison

A job description and an application form can be obtained from the following website:

http://www.imperial.ac.uk/employment/research/index.htm.

Alternatively, please contact Professor Nicholas M Harrison,
Email: nicholas.harrison@imperial.ac.uk.

Completed application forms should be sent to:

Professor Nicholas M Harrison, Department of Chemistry, Exhibition Road,
Imperial College London, SW7 2AZ, U. K.

Closing date: 5 August 2005

Valuing diversity and committed to equality of opportunity.

Postdoctoral Scientist

Nuclear Fuels Simulation and Studies Section
French Atomic Energy Commission at Cadarache

The Nuclear Fuels Simulation and Studies Section of the French Atomic Energy Commission at Cadarache is offering an opportunity for a postdoctoral scientist to work in the field of atomistic modelling of nuclear materials under irradiation. The aim of this project is to use ab initio methods to study the transport properties of fission products in actinide compounds as well as in other nuclear ceramics such as SiC.

This is a one-year appointment with a possibility of a one-year extension and will start in October 2005 or as soon as possible thereafter.

The Cadarache research institute is a interdisciplinary centre located in South-eastern France, approximately 40 km from Aix-en-Provence. The post-doctoral student will join a mixed computational and experimental team, and will be given the opportunity to take part in transport experiments using ion or photon beams. The laboratory has outstanding computational facilities: local PC-clusters and workstations, as well as access to the CEA supercomputing centre.

The candidate should have a Ph. D in computational physics, chemistry or materials science. A strong background in the theory of the electronic structure of solids and good computational skills are required. Prior experience in the use of first-principles methods, in particular Density Functional Theory, would be an advantage.

Applicants can contact Michel Freyss (michel.freyss@cea.fr) or Marjorie Bertolus (marjorie.bertolus@cea.fr) for a detailed job description and an application form. They should submit a detailed resume, including a description of their research achievements and interests.

Ph. D. Studentship

"Computational Materials Design"

Max-Planck-Institute for Iron Research Düsseldorf, Germany

A position for a PhD student in the department "Computational Materials Design" at the "Max-Planck-Institute for Iron Research" in Düsseldorf, Germany is available. The research will be focused on the development and application of ab-initio based multiscale methods to accurately describe structure and electronic properties of interfaces and interfacial defects in modern wide band gap semiconductors.

The main focus will be on nitride-based III-V semiconductors as presently used e.g. to make efficient light emitting devices or as needed for the next generation of DVD players. The research will be performed in close collaboration with experimental and theoretical partners within the EC. Strong interaction with the other groups is therefore expected. The successful candidate should have a degree in Physics, Chemistry or Materials Science, and have a strong interest on microscopic simulations. Preference will be given to candidates with strong background in any (or several) of these fields: electronic structure calculations, molecular modeling, density functional theory, or empirical potentials. The position is funded by the European Research Training Network: "Interfacial Phenomena at Atomic Resolution and multiscale properties of novel III-V SEMiconductors" (PARSEM). The position is reserved to citizens of European Union or of an Associated State (Bulgaria, Iceland, Israel, Liechtenstein, Norway, Romania, Switzerland, and Turkey). German citizens or long-term residents are excluded. Interested candidates should send a CV, list of publications, and name and address (including email) of three references, preferably by email or fax, to:

Prof. Jörg Neugebauer
e-mail: neugebauer@mpie.de
or Dr. Liverios Lymperakis
e-mail: lymperakis@mpie.de

Postal address:
Abteilung "Computergestütztes Materialdesign"
Postfach 140444
40074 Düsseldorf
Germany

Phone: +49 211 6792-286
Fax: +49 211 6792-440

Postdoctoral Positions at MolNaC

(Modeling Laboratory for Nanostructure and Catalysis) Department of Chemistry, University of Salerno, Salerno, Italy

An exceptional PostDoc candidate is required to carry out a collaborative research project involving MolNaC and an experimental group (Prof. Gaetano Guerra) entitled: "Simulations of Nanoporous Polymeric Materials for Hydrogen Storage".

The project involves the development and application of new molecular simulation methods to nanoporous polymeric materials.

Experience in modifying and writing Monte Carlo and/or Molecular Dynamics (not simply using packages) and expertise in the maintenance of computer clusters is required. The initial appointment is for one year (4 months +8 after a positive evaluation of the candidate) with the possibility of a yearly renewal thereafter. The research group has good computational facilities, and friendly atmosphere Computational facilities at Molnac include local workstations, two beowulf cluster, and access to large computer resources via membership at the main supercomputer centres in Europe.

Please send a CV and names of 3 references to Dr. Giuseppe Milano (gmilano@unisa.it).

Research Associate (3 year fixed term)

£20,235 - £22,111 per annum

Department of Mathematical Sciences, Loughborough University, U. K.

Applications are invited for a Postdoctoral Researcher to work on the EPSRC funded project "A multiscale modelling approach to engineering functional coatings". The post will commence on 1st October 2005 (or as soon as possible thereafter) and will be for three years duration.

The aims of the project are to develop models that describe the deposition and growth of functional coatings and to characterise both their optical and mechanical properties. To achieve these aims the project needs to bridge both time and length scales. This will be achieved through the use of techniques from ab-initio methods through to finite-element methods and by the use of long time scale dynamics techniques. This ambitious project will be achieved through collaboration between Loughborough University, Cambridge University, Imperial College London, Newcastle University and the University of Reading.

The particular focus of this post will be in the development of novel potentials to describe both metallic and ionic systems, the interfaces between these materials and their surfaces from ab-initio methods. The post holder will also be expected to perform work on modelling transitions on surfaces that are important to surface growth. The nature of the work will require collaboration both with colleagues at Loughborough University and the other four sites in the project. This will involve several visits to the other sites in the project.

Applicants should have, or shortly expect to receive, a Ph. D. in a relevant field. Experience of undertaking research in the application of density functional theory methods to problems in materials science and the ability to work independently on research problems is essential.

Informal enquiries can be made to: Dr S D Kenny or Professor Roger Smith, e-mail: S.D.Kenny@lboro.ac.uk, R.Smith@lboro.ac.uk; see also `http://www-staff.lboro.ac.uk/~masdk/`

Application forms and further particulars are available from Steven Kenny, Mathematical Sciences, Loughborough University, Loughborough LE11 3TU, UK, Tel: (0)1509 222860, e-mail: S.D.Kenny@lboro.ac.uk , Quote reference: MA/11844. Alternatively an application form can be downloaded from

http://www.lboro.ac.uk/admin/personnel/appform.html.

Curriculum Vitae will only be accepted if accompanied by a completed University application form.

Closing Date: 4 August 2005.

Lecturer or Research Associate Position

Institute of Physics, University of Tsukuba

Research area: Computational bio- and material-science
Term: Until the end of March, 2007
Salary: in the range of about Yen 4,500,000 - Yen 6,000,000, depending on the experience

This position is an official lecturer or research-associate position in National Universities in Japan so that the salary is subject to taxes and regulations of the government. Housing with inexpensive rates shall be provided by the government upon request. Medical-insurance system managed by the government is also applicable to this position.

Research topics: Clarification of atomic and electronic structures of nano- and bio-materials using density functional theory and its beyond. Clarification of the relation between structural transformation and occurrence of functions in proteins or nucleic acids is one of the main topics.

Application: send the following documents to Atsushi Oshiyama via postal mail; (1) Curriculum Vitae, (2) Publications List, (3) Summary of the Accomplishments in the past, (4) (not more than 5) Reprints of the publications, (5) At least one recommendation letter.

Deadline of application: August 12, 2005.

In University of Tsukuba, a special research project on Nanoscience has been and will be conducted during the period between 2002 and 2007. This appointment is for performing a research project in this field using approaches typical of the computational sciences. Members of the research group are Atsushi Oshiyama (Professor), Kenji Shiraishi (Associate Professor), Mauro Boero (Associate Professor) and Masaru Tateno (Associate Professor). Collaborations with (one of) those members are strongly encouraged.

Contact Information:

Atsushi Oshiyama, Institute of Physics, University of Tsukuba, 1-1-1 Tennodai Tsukuba 305-8571, Japan. Phone: +81-29-853-5908, e-mail: oshiyama@comas.frsc.tsukuba.ac.jp

Mauro Boero, Institute of Physics, University of Tsukuba, 1-1-1 Tennodai Tsukuba 305-8571, Japan. Phone: +81-29-853-5921, e-mail: boero@comas.frsc.tsukuba.ac.jp

Pst-doctoral Position

University of Erlangen-Nürnberg, Germany

A post-doctoral position in theoretical solid state physics is available in the Solid state theory group at the University of Erlangen-Nürnberg, Germany.

The research project comprises the density-functional-theory studies of the electron correlation effects on surfaces, in particular, the metallized SiC surface as well as the SiC/graphite interface. The project also involves a study of electron excitations in a framework of time-dependent density functional theory. An adequate knowledge of DFT, many-body theory, as well as the background in a computational solid-state physics is required.

The salary is at the BAT IIa level common at German public universities.

For further information visit our website at

http://www.tfkp.physik.uni-erlangen.de/.

The position is immediately available. Further inquiries and applications (including a CV, names and addresses of three references, summary of research interests, and list of publications) should be directed to Prof. Dr. Oleg Pankratov (Oleg.Pankratov@physik.uni-erlangen.de).

Postdoctoral Position in Computational Materials Theory

Carnegie Institution of Washington, Washington, DC 20015, USA

Applications are solicited for a postdoctoral associateship at the Carnegie Institution of Washington, Washington D.C. to study ferroelectrics using molecular dynamics and first-principles methods. The goal research is to understand high electromechanical coupling piezoelectrics such as PMN-PT and PZN-PT, and to work towards computational materials design to develop new materials with desirable electromechanical properties. A multiscale approach is necessary to span the length and time scales needed to understand relaxor ferroelectrics. The current approach is to fit potential models to first-principles results and perform molecular dynamics simulations. Further abstraction to larger length and longer time scales is also envisioned as part of this project.

Applicants must be familiar with ab-initio density-functional methods and/or molecular dynamics. Facility with FORTRAN is essential and with MPI is desirable. Applicants should send a vita, bibliography, and 3 letters of reference to cohen@gl.ciw.edu. The Carnegie Institution is an Equal Opportunity Employer.

Ronald Cohen
Geophysical Laboratory, Carnegie Institution of Washington
5251 Broad Branch Rd., N.W.
Washington, D.C. 20015
http://www.gl.ciw.edu/~cohen/

Postdoctoral Position
SISSA - Trieste, Italy

A postdoctoral level position is available at the International School for Advanced Studies (Trieste, Italy), starting immediately. The research topic is: Theory of structural, electronic, magnetic and transport properties of metallic nanowires and nanocontacts.

The research will involve the application and development of "ab-initio" methods for the study of the properties of nanowires and nanocontacts particularly of metals with inclusion of the effects of spin-orbit coupling.

The successful candidate should have a PhD in Physics, Chemistry, Material Science or related disciplines and have a good background in electronic structure calculations.

The position is initially for one year, with renewal to a second year subject to success or even beyond subject to availability of funds. The salary will be set according to standard SISSA rules. Pending formal selection procedures, interested candidates should informally send their CV, list of publications, and arrange for at least two reference letters, preferably by email, to:

Prof. Erio Tosatti
and Prof. Andrea Dal Corso
SISSA
e-mail: tosatti@sissa.it
e-mail: dalcorso@sissa.it
Fax: +39/040/3787528

Postdoctoral position in Computational Materials Physics
Materials Department, University of California, Santa Barbara

A postdoctoral position in Computational Materials Physics is available in the Materials Department at the University of California, Santa Barbara. The project involves density-functional theory and GW calculations of bulk and surface defects for materials that may include wide-band-gap semiconductors and oxides (GaN, ZnO, In_2O_3, Ga_2O_3, SnO_2, TiO_2). The postdoc will work jointly with Prof. Chris Van de Walle and Prof. Matthias Scheffler, who is a Distinguished Visiting Professor at UCSB.

Candidates should have experience with electronic structure theory and condensed matter theory. They should also have a keen interest in materials physics and a motivation to interact with experimentalists. Applications should include: (1) Curriculum Vitae, (2) Publication List, (3) One-page summary of accomplishments to date, and their significance, (4) Names and contact information (including email) of three references.

More information about the University of California, Santa Barbara, and about the Materials Department can be found at http://www.ucsb.edu/ and http://www.materials.ucsb.edu/.

Information about the Van de Walle and Scheffler research groups can be found at

`http://www.mrl.ucsb.edu/~vandewalle`

and

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

For more information or to apply, please contact Prof. Chris Van de Walle (vandewalle@mrl.ucsb.edu).

5 Abstracts

Characterization of FePd bilayers and trilayers using soft x-ray resonant magnetic scattering and micromagnetic modeling

G. Beutier
DRFMC, CEA-Grenoble, 17 avenue des Martyrs, 38054 Grenoble, France
G. van der Laan
Magnetic Spectroscopy, Daresbury Laboratory, Warrington WA4 4AD, UK
K. Chesnel, A. Marty, M. Belakhovsky
DRFMC, CEA-Grenoble, 17 avenue des Martyrs, 38054 Grenoble, France
S. P. Collins, E. Dudzik
Magnetic Spectroscopy, Daresbury Laboratory, Warrington WA4 4AD, UK
J.-C. Toussaint
Laboratory Louis Néel, CNRS, PB 166, Grenoble Cedex 9, France
B. Gilles
LTPCM, INPG, BP 75, 38402 Saint Martin d'Hères Cedex, France

Abstract

We have studied bilayers and trilayers of FePd thin-film alloys, where each of the constituting layers has a different magnetic anisotropy, as controlled by the growth conditions. The competition between the magnetocrystalline anisotropy and the shape anisotropy in these films leads to the formation of stripe domains with a period of ∼100 nm, which has been imaged by magnetic force microscopy (MFM). The average magnetic anisotropy has been obtained from the in-plane and perpendicular magnetic field dependence, measured using vibrating sample magnetometry (VSM). We measured the soft x-ray resonant magnetic scattering (SXRMS) at the Fe L_3 edge using σ linearly polarized light, which is sensitive to the magnetization profile in the layers. The magnetic configuration of the layer systems was modelled using micromagnetic software (GL_FFT, ©CNRS). The results of this modeling were used for a numerical simulation of the reflectivity scan and the magnetic rod scans of the SXRMS. This allowed us to determine parameters, such as the lateral roughness, the magnetic period, the magnetic correlation length and the magnetic layer thickness. The good agreement obtained with the experimental results demonstrates that SXRMS provides in-depth information that can not be obtained from either MFM or VSM.

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Impurity and boundary effects in one and two-dimensional inhomogeneous Heisenberg antiferromagnets

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Abstract

We calculate the ground-state energy of one and two-dimensional spatially inhomogeneous antiferromagnetic Heisenberg models for spins 1/2, 1, 3/2 and 2. Our calculations become possible as a consequence of the recent formulation of density-functional theory for Heisenberg models. The method is similar to spin-density-functional theory, but employs a local-density-type approximation designed specifically for the Heisenberg model, allowing us to explore parameter regimes that are hard to access by traditional methods, and to consider complications that are important specifically for nanomagnetic devices, such as the effects of impurities, finite-size, and boundary geometry, in chains, ladders, and higher-dimensional systems.

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Effects of nanoscale spatial inhomogeneity in strongly correlated systems

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Abstract

We calculate ground-state energies and density distributions of superlattices characterized by periodic modulations of the on-site interaction and the on-site potential. Both density-matrix renormalization group and density-functional methods are employed and compared. We find that small variations in the on-site potential v_i can simulate, cancel, or even over-compensate effects due to much larger variations in the on-site interaction U_i. Our findings highlight the importance of nanoscale spatial inhomogeneity in strongly correlated systems, and call for reexamination of model calculations assuming spatial homogeneity.

(Phys. Rev. B **71**, p. 125130 (2005))

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Energy lowering of current-carrying single-particle states in open-shell atoms due to an exchange-correlation vector potential

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Abstract

Current-density-functional theory is used to perturbatively calculate single-particle energies of open-shell atoms prepared in a current-carrying state. We focus on the highest occupied such energy, because its negative is, in principle, the exact ionization energy. A variety of different density functionals and calculational schemes are compared with each other and experiment. When the atom is prepared in a current-carrying state, a current-dependent exchange-correlation functional is found to slightly lower the single-particle energy of the current-carrying orbital, as compared to a calculation using standard (current independent) density functionals for the same system. The current-dependent terms in the exchange-correlation functional thus provide additional stabilization of the current-carrying state.

(Int. J. Quantum Chem. **103**, p. 516 (2005); proceedings of 2004 SBQT meeting)
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Spin-density-functional theory: some open problems and application to inhomogeneous Heisenberg models

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Abstract

Spin-density-functional theory (SDFT) is the most widely implemented and applied formulation of density-functional theory. However, it is still finding novel applications, and occasionally encounters unexpected problems. In this paper we first briefly describe a few of the latter, related to issues such as nonuniqueness, noncollinearity, and currents. In the main part we then turn to an example of the former, namely SDFT for the Heisenberg model. It is shown that time-honored concepts of *ab initio* DFT, such as the local-density approximation, can be applied to this (and other) model Hamiltonians, too, once the concept of 'density' has been suitably reinterpreted. Local-density-type approximations for the inhomogeneous Heisenberg model are constructed. Numerical applications to finite-size and impurity systems demonstrate that DFT is a computationally efficient and reasonably accurate alternative to conventional methods of statistical mechanics for the Heisenberg model.

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Density-functional treatment of model Hamiltonians: basic concepts and application to the Heisenberg model

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Abstract

We describe how density-functional theory, well-known for its many uses in *ab initio* calculations of electronic structure, can be used to study the ground state of inhomogeneous model Hamiltonians. The basic ideas and concepts are discussed for the particular case of the Heisenberg model. As representative applications, illustrating scope and limitations of the procedure, we calculate the ground-state energy of one-, two- and three-dimensional antiferromagnetic Heisenberg models in the presence of boundaries and of impurities in the bulk and at the surfaces. Correlations are shown to lift degeneracies present in the mean-field approximation. Comparison with exact (brute force) diagonalization shows that the density-functional results are a significant improvement over the mean-field ones, at negligible extra computational cost

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First-principle Wannier functions and effective lattice fermion models for narrow-band compounds

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Abstract

We propose a systematic procedure for constructing effective lattice fermion models for narrow-band compounds on the basis of first-principles electronic-structure calculations. The method is illustrated for the series of transition-metal (TM) oxides: $SrVO_3$, $YTiO_3$, V_2O_3, and $Y_2Mo_2O_7$, whose low-energy properties are linked exclusively to the electronic structure of an isolated t_{2g} band. The method consists of three parts, starting from the electronic structure in the local-density approximation (LDA). (i) construction of the kinetic-energy Hamiltonian using formal downfolding method. It allows to describe the band structure close to the Fermi level in terms of a limited number of (unknown yet) Wannier functions (WFs), and eliminate the rest of the basis states. (ii) solution of an inverse problem and construction of WFs for the given kinetic-energy Hamiltonian. Here, we closely follow the construction of the basis functions in the liner-muffin-tin-orbital (LMTO) method, and enforce the orthogonality of WFs to other bands. In this approach, one can easily control the contributions of the kinetic energy to the WFs. (iii) calculation of screened Coulomb interactions in the basis of *auxiliary* WFs. The latter are defined as the WFs for which the kinetic-energy term is set to be zero. Meanwhile, the hybridization between TM d and other atomic states is well preserved by the orthogonality condition to other bands. The use of auxiliary WFs is necessary in order to avoid the double counting of the kinetic-energy term, which is included explicitly in the model Hamiltonian. In order to calculate the screened Coulomb interactions we employed a hybrid approach. First, we evaluate the screening caused by the change of occupation numbers and the relaxation of the LMTO basis functions, using the conventional constraint-LDA approach, where all matrix elements of hybridization connecting the TM d orbitals and other orbitals are set to be zero. Then, we switch on the hybridization and evaluate the screening of on-site Coulomb interactions associated with the change of this hybridization in the random-phase approximation. The second channel of screening appears to be very important, and results in relatively small value of the effective Coulomb interaction for isolated t_{2g} bands (about 2-3 eV, depending on the material). We discuss details of this screening and consider its band-filling dependence, frequency dependence, influence of the lattice distortion, proximity of other bands, as well as the effect of dimensionality of the model Hamiltonian.

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Effect of post-growth annealing on the optical properties of InAs/GaAs quantum dots: A tight-binding study

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Abstract

We present an atomistic study of the changes of the strain field, the one-particle electronic spectrum and the oscillator strength of the fundamental optical transition in $In_xGa_{1-x}As$ pyramidal quantum dots (QDs) due to interdiffusion, using a combination of Keating's valence force field (VFF) and empirical tight-binding (ETB). We find that the transition energy is significantly affected by both the chemical effect of interdiffusion and the concomitant strain relief inside the QD. Our results are in agreement with recent luminescence studies of intermixed QDs.

(submitted to: Phys. Rev. Lett.)
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Theory of Photoemission Spectra of Actinide Compounds

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Abstract

The photoemission spectra of actinide compounds are modelled by a dynamical mean field theory. The complete multiplet spectrum of a single ion is calculated by exact diagonalization of the two-body Hamiltonian of the f^n shell. A coupling to auxiliary fermion states models the interaction with a conduction sea. The ensuing self-energy function is combined with a band Hamiltonian of the compound, calculated in the local-density approximation, to produce a solid state Green's function. The theory is applied to PuSe and elemental Am. For PuSe a sharp resonance at the Fermi level arises from mixed valent behavior, while several features at larger binding energies can be identified with quantum numbers of the atomic system. For Am the ground state is dominated by the $|f^6; J = 0\rangle$ singlet but the strong coupling to the conduction electrons mixes in a significant amount of f^7 character.

(Phys. Rev. Lett.: submitted)
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Ab initio tight-binding LMTO method for nonequilibrium electron transport in nanosystems

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Abstract

We present an *ab initio* method for calculation of the electronic structure and electronic transport of nanoscale systems coupled to electrodes with applied voltage bias. The method is based on the local density approximation of density functional theory and implemented in the framework of the tight-binding linear muffin-tin orbital approach in its atomic sphere approximation. A fully atomistic description of the electrodes and the nanosystem is used, and the self-consistent charge and electrostatic potential for the system under applied bias is calculated using the nonequilibrium Green's function (NEGF) approach. General expressions for the lesser Green's function and transmission coefficient obtained within NEGF theory are rewritten using auxiliary Green's functions that are defined by the inverse of the short-ranged structural constants. This reformulation of the theory with auxiliary Green's functions allows the use of very effective and well-developed tight-binding techniques. The method is applied to three systems: a single benzene di-thiol molecule coupled to (111) gold electrodes, a single gold atom coupled to (100) gold electrodes, and a single platinum atom coupled to (100) platinum electrodes.

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6 SCIENTIFIC HIGHLIGHT OF THE MONTH: Diluted Magnetic Semiconductors

Dilute Magnetic Semiconductors

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Abstract

We describe exchange interactions in dilute magnetic semiconductors (DMS) based on ab-initio calculations. Electronic structure of DMS is calculated on the basis of the density functional theory by using the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA). We will show that there are two classes of DMS with very different properties. In systems with localised majority d-states deep in the valence band, the ferromagnetism is induced by Zener's p-d exchange interaction. This interaction is weak but long ranged. For systems with impurity-bands in the gap, the ferromagnetism is driven by Zener's double exchange mechanism. This interaction is very strong but short ranged. Sophisticated Monte Carlo methods show that for small concentrations the percolation effect should be included to estimate Curie temperatures of DMS. In particular, the ferromagnetism is strongly suppressed in double exchange systems due to the absence of the percolation for low concentrations.

1 Introduction

Half-metals are considered to be the ideal materials for spintronics. They are particular ferromagnets which from electronic structure point of view can be considered as hybrids between metals and semiconductors, since the majority density of states is metallic, i.e., finite at the Fermi level E_{F}, while the minority bands exhibit a gap at E_{F}. Therefore at E_{F} a 100 % spin polarisation exists, which is ideal for the efficiency of spin dependent devices [1, 2].

Since the discovery of half-metallicity in the Heusler alloys by de Groot [3], many other materials like certain manganites, e.g., $La_{0.7}Sr_{0.3}MnO_3$ [4], double perovskites, e.g., Sr_2FeReO_6 [5] as well as the transition metal oxides CrO_2, Fe_2O_3 [4] have been shown to be half-metals. To this class also belong dilute magnetic semiconductors (DMS), such as $In_{1-x}Mn_xAs$ and $Ga_{1-x}Mn_xAs$ discovered by Munekata et al. [6] and Ohno et al. [7]. In these systems a small concentration of

Mn atoms, or in general of transition metal atoms (TM), with typical concentrations of 3 - 8 %, are randomly distributed on the cation sites. Due to the small concentrations the systems behave structurally as semiconductors and can be easily grown on the corresponding parent substrate, i.e., (Ga, Mn)As on GaAs. Moreover they can be doped and manipulated as semiconductors, which offers a large prospect for applications. However a problem of these DMS-systems is, that the Curie temperatures are well below room temperature, e.g., 170 K for (Ga, Mn)As, representing the best investigated system. This is the major obstacle for applications [1, 2, 8].

In this paper, we will discuss the basic electronic structure of dilute magnetic semiconductors. We will concentrate on the magnetic properties, in particular the exchange mechanism which control the ferromagnetism in these systems. Moreover we present calculations of the Curie temperatures based (i) on the most simple mean-field approximation and (ii) on sophisticated Monte Carlo methods. The ab-initio calculations are performed within the density functional formalism by using the Korringa-Kohn-Rostoker (KKR) method together with the coherent potential approximation (CPA) to describe the disorder in these systems. As a result we will show that there are two classes of DMS, one, in which the majority d-states are well localised below the valence band, and a second one, where impurity d-bands in the gap exist. In the former class the interaction is dominated by Zener's p-d exchange being relatively weak, but longer ranged, while in the latter one Zener's double exchange prevails, being strong but short ranged. Both have important consequences for the Curie temperatures.

2 Ab-initio Calculations for Dilute Magnetic Semiconductors

The results presented in this review are obtained by ab-initio calculations based on density functional theory (DFT). Exchange and electronic correlation effects are described by the local density approximation, the standard working horse in the field. As calculational method we use the KKR-Green function method. Green function methods avoid the calculation of eigenfunction ϕ_α and eigenvalues E_α of the Kohn-Sham equations of DFT. The Green function $G(\boldsymbol{r}, \boldsymbol{r}'; E)$, defined as the causal solution of the Kohn-Sham equation with a unit source term at the position $\mathbf{r}'$

$$(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) - E)G(\boldsymbol{r}, \boldsymbol{r}'; E) = -\delta(\boldsymbol{r} - \boldsymbol{r}') \tag{1}$$

allows to determine the charge density $n(\boldsymbol{r})$ directly from its imaginary part by integrating over all occupied states

$$n(\boldsymbol{r}) = -\frac{2}{\pi}\int^{E_\mathrm{F}} dE \mathrm{Im}G(\boldsymbol{r}, \boldsymbol{r}; E) \tag{2}$$

and the density of states (DOS) in a certain volume V by a volume integral

$$n(E) = -\frac{2}{\pi}\int_V d\boldsymbol{r} \mathrm{Im}G(\boldsymbol{r}, \boldsymbol{r}; E) \tag{3}$$

The KKR method is based on multiple scattering theory which is of strong advantage for the description of the disorder introduced by the transition metal impurities like Mn, which are

randomly distributed on the cation sites, i.e., on the Ga sites in GaAs. Therefore this disorder corresponds to the disorder in a random A_cB_{1-c} alloy where $c = c_A$ denotes the concentration of A atoms and $c_B = 1 - c_A$ the one of B atoms. This disorder problem can be well described by the coherent potential approximation (CPA) [9], in which the atoms A and B are embedded in an effective 'CPA'-medium which is determined selfconsistently. If we denote the atomic t-matrices of the A- and B-atoms and of the CPA medium by t_A, t_B and t_{CPA}, then the CPA selfconsistency condition, which determine t_{CPA}, leads in the multiple scattering KKR description to

$$c_A T_A + c_B T_B = 0 \tag{4}$$

where $T_{A,B}$ describes the total single-site T-matrix of an atom A or B embedded in the CPA medium on site 0

$$T_A = (t_A - t_{CPA}) \frac{1}{1 - G^{00}_{CPA}(t_A - t_{CPA})} \tag{5}$$

where G^{00}_{CPA} are the on-site elements of the CPA Green function G_{CPA} at site 0. These elements can be calculated from t_{CPA} by Brillouin zone integration

$$G_{CPA} = \frac{1}{V_{BZ}} \int_{BZ} d\boldsymbol{k} g(\boldsymbol{k}) \frac{1}{1 - t_{CPA} g(\boldsymbol{k})} \tag{6}$$

where $g(\boldsymbol{k})$ are the free space structure constants.

According to eq. (5) the CPA medium, i.e., the CPA-scattering matrix t_{CPA}, has to be chosen such that on the statistical average the insertion of an A and B atom at the considered site into the CPA medium does not change the scattering which is the condition of eq. (4). In our calculations we used the KKR-CPA code MACHIKANEYAMA 2000 produced by H. Akai of Osaka University [10].

All the above considerations can be easily generalised to the case of a spin polarised system where we have to distinguish two charge densities $n^+(\boldsymbol{r})$ and $n^-(\boldsymbol{r})$, where $n(\boldsymbol{r}) = n^+ + n^-$ and $m(\boldsymbol{r}) = n^+ - n^-$ are the charge- and magnetisation-densities. All quantities G, t_A, t_B, T_A etc. have then an additional spin index. For dilute magnetic semiconductors it is very important to distinguish two states, the ferromagnetic one, where all moments of the magnetic atoms are aligned in one direction, or the disordered-local-moment (DLM) state (or spin-glass state) where the directions of all local moments are randomly distributed, so that the average magnetisation vanishes. While the description of the ferromagnetic states is straightforward in the above CPA formalism, the DLM state can be considered as a three component alloy, where in addition to the Ga atoms with concentration $1 - c$, the Ga sites are occupied either with Mn atoms with local moment 'up' ($Mn^{\uparrow}$) or with Mn atoms with moment 'down' ($Mn^{\downarrow}$), both with equal concentrations $c/2$ [9].

To evaluate the thermodynamic properties, we describe the system by a classical Heisenberg model

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \vec{M}_i \cdot \vec{M}_j \tag{7}$$

where $\vec{M}_i$ and $\vec{M}_j$ denote the local moments, in particular their directions, of the magnetic impurities i and j and J_{ij} the exchange integral between these atoms. This we calculated by the formula of Liechtenstein [11], which describes the energy change due to a small change of the angle between both moments within the frozen potential approximation.

$$J_{ij} = \frac{1}{4\pi}\mathrm{Im}\int^{E_\mathrm{F}} dE \mathrm{Tr}\{(t_i^+ - t_j^-)G_{ij}^+(E)(t_i^+ - t_j^-)G_{ji}^-(E)\} \tag{8}$$

$t_i^\pm$ is the atomic t-matrix of atom i for majority(+) and minority(-) spin directions and $G_{ij}^\pm$ is the Green function of the system.

The disorder of the other atoms is described by identifying the Green function $G_{ij}^\pm$ between i and j by the Green function of the ferromagnetic CPA medium. The exchange coupling constants J_{ij} describe not only the sign and the strength of the coupling, but also their spatial extent, which is particular important for the considered diluted systems.

Given the J_{ij}, the thermodynamic properties and in particular the Curie temperature T_C can be described by standard statistical methods. In the simplest mean-field approximation (MFA) the action of all neighbors j of impurity i is calculated by an average field

$$H_i = c\sum_{j(\neq i)} J_{ij}\langle M_j\rangle \tag{9}$$

where $\langle M\rangle = \langle M_j\rangle = \langle M_i\rangle$ is the average moment and c the occupation probability for site j. The condition of vanishing $\langle M\rangle$ then yields as Curie temperature in MFA

$$k_\mathrm{B}T_\mathrm{C}^\mathrm{MFA} = \frac{1}{3}cM^2\sum_{j(\neq i)} J_{ij} \tag{10}$$

Note that in MFA only the sum of all J_{ij} enters, but not the spatial extent. Therefore the mean-field value $T_\mathrm{C}^\mathrm{MFA}$ can also be calculated directly from the CPA total energies for the ferromagnetic ground state E_FM and from the disordered local moment state E_DLM. In the mean-field approximation of the Heisenberg model the ground state energy H_DLM vanishes for the DLM states

$$H_\mathrm{DLM} = -\frac{1}{2}\sum_{i\neq j} J_{ij}\langle M_i\rangle\cdot\langle M_j\rangle = 0 \tag{11}$$

since the average moments $\langle M_i\rangle$ vanish due to the average over all directions. On the other hand for the ferromagnetic ground state one obtains:

$$H_\mathrm{FM} = -\frac{1}{2}c^2M^2\sum_{i\neq j} J_{ij} \tag{12}$$

Since orientational degrees of freedom should be described well by the Heisenberg model, we can identify the difference

$$H_\mathrm{DLM} - H_\mathrm{FM} = E_\mathrm{DLM}^\mathrm{CPA} - E_\mathrm{FM}^\mathrm{CPA} \tag{13}$$

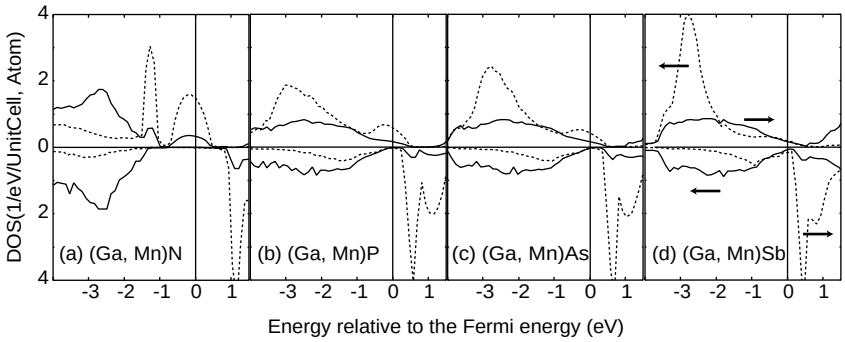

Figure 1: Density of states of dilute magnetic semiconductors with 5 % Mn impurities: (a) (Ga, Mn)N, (b) (Ga, Mn)P, (c) (Ga, Mn)As and (d) (Ga, Mn)Sb. The full curve gives the average DOS of the whole system, the dotted curve the local DOS of the Mn atoms.

by the total energy difference for the ferromagnetic system, e.g., $Ga_{1-c}Mn_c^{\uparrow}As$, and the DLM system with 50 % Mn moments up and 50 % down, i.e., $Ga_{1-c}Mn_{c/2}^{\uparrow}Mn_{c/2}^{\downarrow}As$. By comparison with the above result for T_C^{MFA} we obtain then

$$k_B T_C^{MFA} = \frac{2}{3} \frac{E_{DLM}^{CPA} - E_{FM}^{CPA}}{c} \tag{14}$$

Thus in MFA the Curie temperature is determined by the total energy difference per Mn atom between the DLM and FM state [12].

Often the MFA does not give reliable results. In this case Monte Carlo simulations offer an (numerically) exact method to calculate the thermodynamic properties. For details see Sect. 5.

3 Local Density of States and Curie Temperatures in MFA

Here we present results of ab-initio calculations for a series of III-V DMS with 5 % Mn impurities. We have chosen the sequence (Ga, Mn)N, (Ga, Mn)P, (Ga, Mn)As and (Ga, Mn)Sb, where only the anions N, P, As and Sb are different. For the results it is most important that the majority d-level of Mn has a lower energy than the atomic p-level of Sb, but a higher energy than the p-level of N, while the p-levels of P and As are intermediate.

Fig. 1 shows the density of states (DOS) for the considered systems with 5 % Mn on the Ga sites. The upper curves refers to the majority DOS, the lower inverted ones to the minority DOS, both for the ferromagnetic configuration. The full curves show the average total density of states of the DMS with 5 % Mn. Due to the small concentration of Mn this is roughly the DOS of the pure semiconductors, consisting of the occupied valence band, dominated by the anion p-states and the empty conduction band, formed mostly by the Ga s-states. The dotted lines show the local DOS of the Mn atoms. We consider only the neutral charge state without additional dopants. Since Mn has 7 valence electrons and substitutes for a Ga atom, 3 of the 7 electrons can replace the 3 Ga electrons in the valence band. The remaining 4 electrons have to be put in new localised d-states in the band gap. Therefore the electronic structure of transition metal impurities in semiconductors is dominated by d-states in the gap, which for finite concentrations develop into impurity bands. Since Mn has a large moment, only the majority states are occupied leading

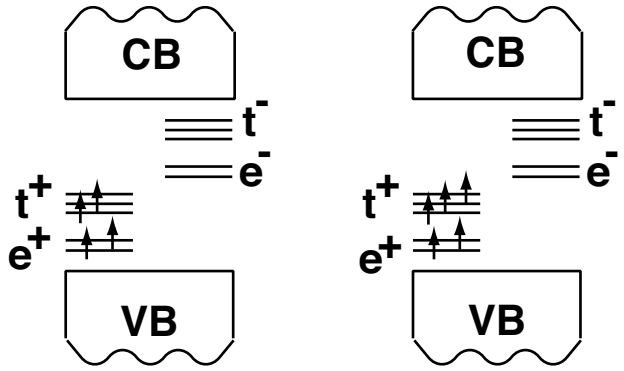

Figure 2: Impurity levels of magnetic transition metal impurities in semiconductors: For Mn on the III-site in III-V semiconductors the double degenerate e^+ state and two of the three degenerate t^+ states are occupied (left figure); the same states are occupied for Cr impurities on II-sites in II-VI semiconductors. On the other hand for Mn impurities in II-VI and Fe impurities in III-V semiconductors all five majority states (right figure) are occupied.

to a so-called 'high-spin state'. The impurity levels are schematically indicated in Fig. 2. Two different impurity levels have to be distinguished: A twofold degenerate e-state ($d_{z^2}, d_{x^2-y^2}$), the wave functions of which for symmetry reasons hybridize very little with the valence band p-states, and a threefold degenerate t-state (d_{xy}, d_{yz}, d_{zx}) which strongly hybridizes with the p-states, resulting in bonding- and antibonding hybrides. While the bonding hybrides are located in the valence band, the antibonding hybrides form the impurity t-states in the gap, which are due to the hybridization shifted to higher energies than the e-states. In the neutral configuration only the two e-states and two of the three t-states in the majority band are occupied, while the minority gap states are empty.

In Fig. 1 both the e- and t-states can be very well seen for the GaN compound with 5 % Mn. Since the d-states around the individual Mn atoms overlap and form an impurity band, the higher and broader band corresponds to the more extended t-states, and the lower narrow one to the more localised e-states. Within the valence band there is also some hybridised-in Mn DOS from the bonding t-hybrides. The Fermi level falls into the majority t-impurity band, such that per Mn atom exactly two e-states and two t-states are occupied, leaving one majority t-state and all minority d-states empty. Therefore the considered system is a half-metallic ferromagnet, with a moment of 4 μ_{B} per Mn atom.

When we move from Mn in GaN to Mn in GaP and GaAs we notice that the Mn d-level is shifted to lower energies. For (Ga, Mn)P the e-state has fully moved in the valence band, while the t-state forms with the valence p-states of the P atom a resonance at E_{F}. Most of the local d-intensity of the Mn atom is now located at the bonding t-states within the valence band. For (Ga, Mn)As these trends are even somewhat stronger. Finally for (Ga, Mn)Sb, the resonance at the Fermi level has more or less disappeared, such that at E_{F} the local Mn DOS agrees well with the DOS of the Sb atoms. Since the minority d-like gap states are in all cases unoccupied, the total moment is fixed to 4 μ_{B} per Mn. However in the case of (Ga, Mn)Sb the situation is very different from (Ga, Mn)N, since in GaSb all 5 majority d-states are occupied, while a hole exist in the Sb majority p-states at the Fermi level. Therefore the filling of the five d-resonances leads to a total moment of 5 μ_{B}, which is, however, reduced to 4 μ_{B} per Mn atom by the empty states in

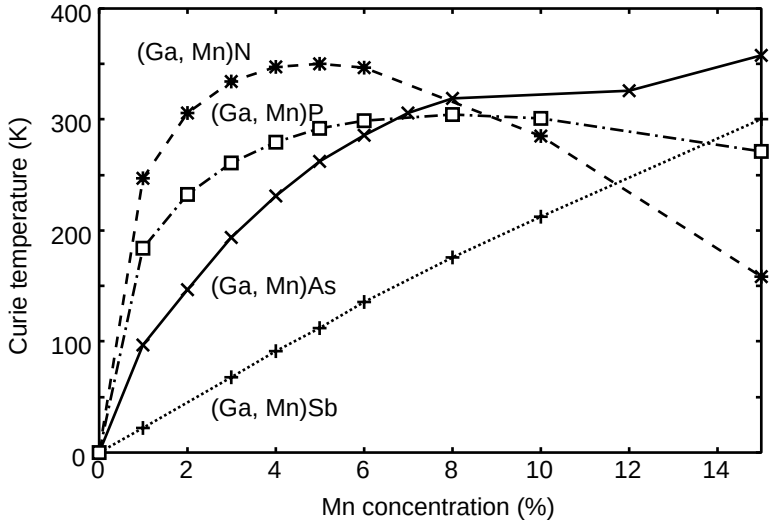

Figure 3: Curie temperatures of Mn doped III-V semiconductors, as calculated in the mean field approximation as a function of the Mn concentration.

the majority p-band. Thus in the CPA description the Sb atoms are weakly and homogeneously polarised, with an average moment of -1 $\mu_{\rm B}$ per Mn atom, being antiferromagnetically coupled to the Mn moments, such that the total moment per Mn atom is still 4 $\mu_{\rm B}$. In summary the behaviour of Mn in GaN and GaSb is completely different. In fact, both systems represent two extremes: in (Ga, Mn)N the d-states are in the gap and form impurity bands at $E_{\rm F}$, while in (Ga, Mn)Sb the d-states are at the lower end of the valence band and fully occupied, while a hole exist in the majority valence band. The behaviour of Mn in GaP and GaAs lies between these two extremes. In all cases the minority d-states are unoccupied.

The Curie temperatures $T_{\rm C}$, calculated in MFA for these systems, reflect this strongly different behaviour. Fig. 3 shows the calculated $T_{\rm C}^{\rm MFA}$ values for the four systems as a function of the concentration c of Mn impurities. For (Ga, Mn)Sb we find a linear dependence on the concentration, but in the other cases a strong non-linear dependence is obtained, which is particular pronounced for (Ga, Mn)N. As we will demonstrate below, in this case $T_{\rm C}^{\rm MFA}$ scales as the square root of the concentration c, leading to very large $T_{\rm C}$ values already for small concentrations of Mn. The behaviour of (Ga, Mn)As is intermediate between these extremes: a weaker $\sqrt{c}$-dependence for smaller concentrations and a linear dependence for larger concentrations. As we will discuss in the following, the different concentration dependences are caused by two different exchange mechanisms, which stabilize the ferromagnetism, i.e., double exchange in the case of impurity bands in the gap and kinetic or p-d exchange in the case of nearly localised d-levels below the valence band [13].

4 Double Exchange, Super Exchange and Kinetic p-d Exchange

To identify the exchange mechanism, which stabilises ferromagnetism or antiferromagnetism, is an important problem in magnetic materials. For dilute magnetic semiconductors this means identifying the mechanism which stabilises the ferromagnetism already for small concentrations [12, 13, 14].

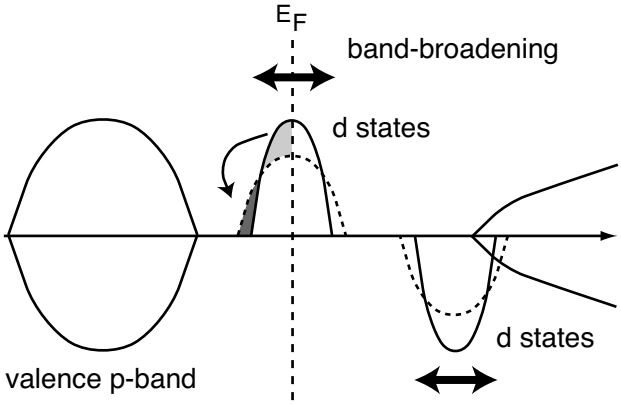

Figure 4: Double exchange: Due to the broadening of the impurity t-band with increasing Mn concentration c, states are transferred to lower energies, leading to an energy gain, if the Fermi energy lies in the band. As explained in the text, the band width increases as $\sqrt{c}$.

For (Ga, Mn)N the characteristic features of the DOS of the ferromagnetic state is sketched in Fig. 4. The Fermi energy lies in the majority impurity band of t-symmetry. The important energy gain arises from the broadening of the impurity band with increasing concentration c. If we increase the concentration from a lower value, with the DOS given by the full line, to a larger value corresponding to the broader DOS as given by the dashed line, we transfer DOS-weight from around $E_{\rm F}$ to lower energies, leading to an energy gain, which, as we will show, stabilises the ferromagnetic state. This energy gain is proportional to the band width W of the impurity band, which scales as the square root $\sqrt{c}$ of the concentration. The energy gain due to band broadening is known as Zener's double exchange [14].

This can be proven by a theorem for tight-binding model. The square of the band width is given by the energy variance

$$W^2 = \overline{(E - \bar{E})^2} = \sum_{m \neq 0} |H_{0m}|^2 \tag{15}$$

which itself is determined by the sum of the hopping probabilities $|H_{0m}|^2$ from site 0 to any other site m. H_{0m} is the so-called hopping matrix element. Consider now a disordered lattice with a random distribution of Mn atoms. Starting from a given Mn atom at site 0, an electron can only hop from the state centered at 0 to the site m, if this site is occupied by another Mn atom. If we denote the Mn-Mn hopping integral by t_{0m}, we find in the disordered system

$$H_{0m} = t_{0m}(\text{if Mn atom at m}) \text{ or } 0(\text{otherwise}) \tag{16}$$

By averaging over all configurations of Mn atoms we therefore obtain

$$\langle W^2 \rangle_{\rm conf} = \sum_{m \neq 0} \langle |H_{0m}|^2 \rangle = c \sum_{m \neq 0} |t_{0m}|^2 \tag{17}$$

since the probability to find a Mn atom at site m is given by the atomic concentration c. Thus the effective band width $W_{\rm eff}$ scales as $\sqrt{c}$. This $\sqrt{c}$ behaviour of band width can be clearly

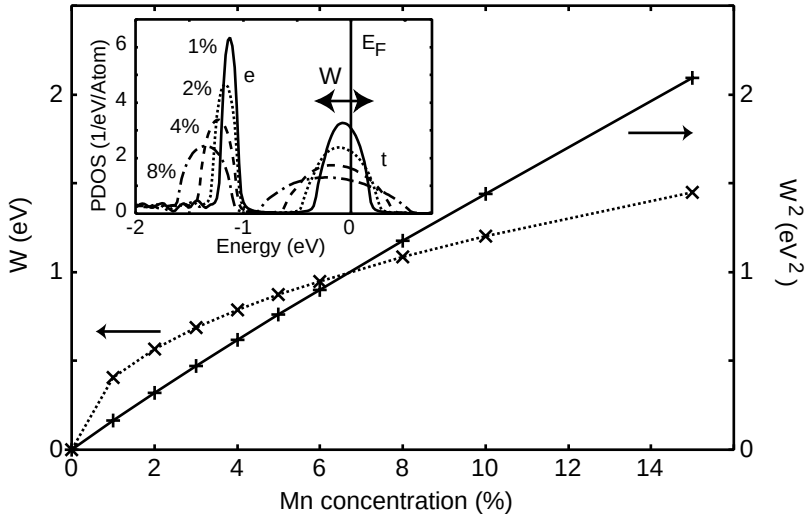

Figure 5: Impurity band width W and its square W^2 for the impurity t-band in (Ga, Mn)N as a function of Mn concentration. The inset shows the local density of Mn gap states.

seen in calculated DOS as is shown in Fig. 5. In the figure W and its square are plotted as a function of Mn concentration. The linear dependence of W^2 on Mn concentration indicates a $\sqrt{c}$ dependence of W. Thus, the energy gain of the ferromagnetic state with increasing concentration scales as $\sqrt{c}$, which explains the strong increase of the Curie temperature in MFA as shown in Fig. 3 for (Ga, Mn)N. The double exchange mechanism is only important, if the Fermi energy lies in the band. If the band is completely occupied or empty, no energy can be gained by band broadening.

Let us now consider the stability of the disordered local moment (DLM) (or spin-glass) state as compared to the ferromagnetic one. In the CPA-description of the DLM state, for a given Mn atom 50 % of the neighboring Mn atoms have a moment being parallel aligned to the central moment, and 50 % are antiferromagnetically aligned. The parallel aligned pairs lead, as in the ferromagnetic case, to a broadened impurity band, but with a reduced band width scaling as $\sqrt{c/2}$, since only 50 % of the pairs are parallel aligned. Therefore in total the double exchange due to band broadening always favors the ferromagnetic configuration.

The 50 % antiferromagnetically aligned pairs gain energy by super-exchange. The density of states in the gap of two Mn impurities with antiparallel aligned moments is schematically shown in Fig. 6. Note that the minority and majority peaks are exchanged for the two atoms. Since the wave functions with the same spin directions hybridise with each other, covalent bonding and antibonding hybrides are formed. From the energetic point of view it is important, that the lower bonding states are shifted to lower energies, while the higher antibonding states are shifted to higher energies. Thus energy is gained by super-exchange, if the Fermi energy is located between the two peaks or in the peaks, however not, if E_{F} is below or above both peaks. As can be shown, the energy gain is given by $c\frac{t^2}{IM}$, where t is the effective hopping matrix element and IM is the exchange splitting, given by the exchange integral I times the local moment M. It is linear in c, since the effects of several antiparallel aligned neighbours on the central atom superimpose on each other.

Thus in the case of impurity bands in the gap, double exchange favors the ferromagnetic config-

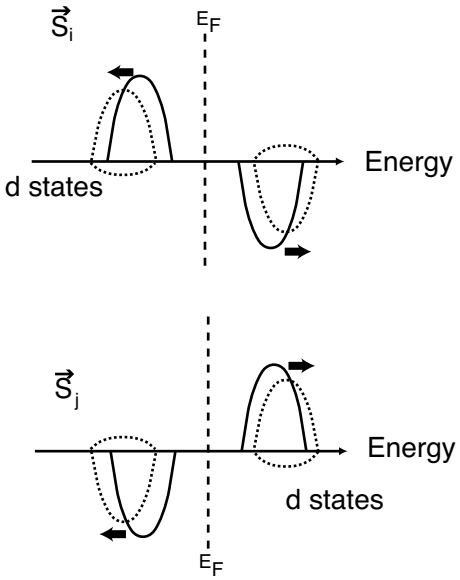

Figure 6: Super exchange: Shown are the local densities of states for two impurities with moments $\vec{S}_i$ = 'up' and $\vec{S}_j$ = 'down'. Due to hybridisation of the majority and the minority d-wavefunctions the lower energy levels are shifted to lower and the higher levels to higher energies as indicated by the dashed lines. Due to hybridisation also small peaks occur locally for the 'wrong' spin direction. The downward shift stabilises the antiferromagnetic alignment of the two local moments, provided the Fermi level falls between the two peaks, but not below or above.

uration and always wins, if the Fermi energy lies (well) in the band. Then the energy gain due to double exchange, scaling as $\sqrt{c}|t|$, is always larger than the energy gain due to super exchange, scaling like $c|t|^2/IM$. However if the Fermi energy lies between the two bands or lies close to the band edges, super exchange wins stabilising the disordered local moment state. Thus the system (Ga, Mn)N is expected to be a ferromagnet, while (Ga, Fe)N should be a disordered system, since the t-band is completely filled. For the same reason, in the II-VI compounds Cr impurities should favour the ferromagnetic state, but Mn impurities the DLM state.

However these considerations are only valid for impurity band systems. If the majority d-level lies below the valence p-states, as it is the case for (Ga, Mn)Sb in Fig. 1, then we have a different situation which is schematically sketched in Fig. 7. In the majority band the low lying d-states of Mn hybridise with the valence band p-states of Sb, and effectively push the majority valence band to higher energy. The opposite is true for the minority valence states being pushed by the empty minority d-states to lower energies. Thus the valence band becomes spin polarised, with a moment of $-1\mu_B$ per Mn atom, i.e., antiparallel to the Mn moment. The other Mn atoms gain energy by also aligning antiparallel to this host polarisation, thus leading to an indirect ferromagnetic coupling of the Mn-atoms. Due to the strong localisation of Mn d wavefunctions the direct d-d interaction is very small.

This kind of exchange interaction is called Zener's kinetic or p-d exchange and favours ferromagnetism. No energy gain is obtained in the DLM state, since the host polarisations induced by non-aligned Mn moments cancel each other.

All ab-initio calculations presented in the previous section are based on the local density ap-

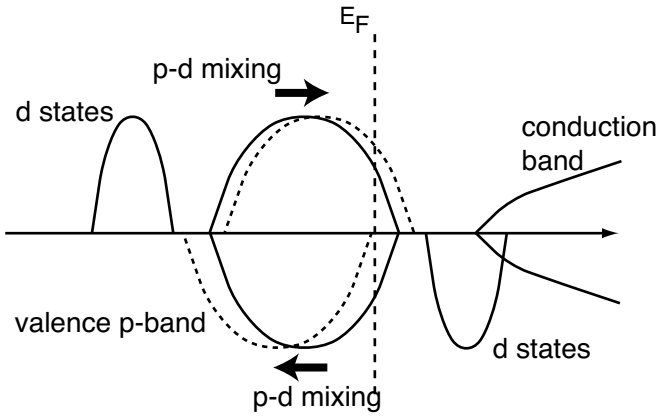

Figure 7: Kinetic p-d exchange: The low-lying 'localised' majority d-states hybridise with the majority valence p-band, pushing it up to higher energies as indicated by the dashed line. Analogously the empty minority d-level pushes the minority valence p-states to lower energies. Since due to charge neutrality the valence band must have one hole per Mn atom, this hole is confined to the majority band, leading to an Sb moment of $-1\mu_{\mathrm{B}}$ per Mn being antiferromagnetically aligned to the Mn-moments.

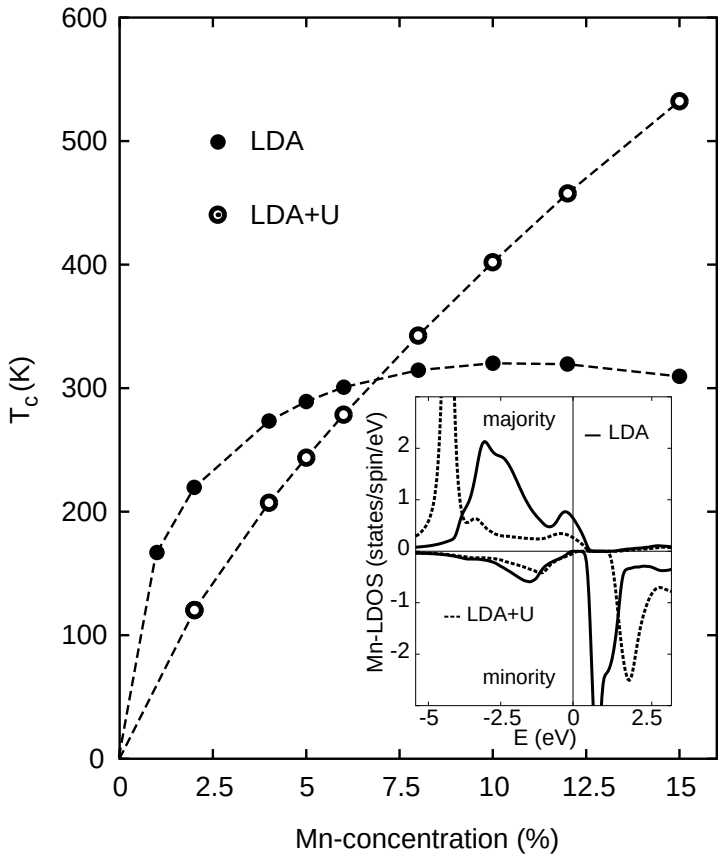

Figure 8: Meanfield Curie temperature of (Ga, Mn)As evaluated in the LDA and in the LDA+U approximation (with $U = 4$ eV). The inset shows the local density of states of the Mn atoms. Due to the Hubbard U of 4 eV, the Mn majority d-states are shifted to lower energies, while the resonance at the Fermi level is diminished. This increases the importance of p-d kinetic exchange and reduces the double exchange, so that T_{C} varies linear with concentration.

proximation (LDA). This approximation works in most cases very well, but has its limit for correlated systems. One typical error is, that the spin splitting is usually too small. The error can be partially removed by the LDA+U method, where U stands for the Hubbard U parameter of the Hubbard model. Fig. 8 shows the results of an LDA and LDA+U calculations for (Ga, Mn)As system with 5 % Mn. The inset shows the local Mn DOS in LDA and LDA+U, using a U parameter of $U = 4$ eV. As one sees, the U parameter of 4 eV shifts the majority peak by about 1.3 eV to lower energies, such that it is in good agreement with photoemission measurements [15, 16]. Since the d-states are now located in the lower region of the valence band, one expects that the p-d exchange becomes more dominant. The calculated Curie temperatures $T_{\mathrm{C}}^{\mathrm{MFA}}$ indeed show this effect. The LDA results show a $\sqrt{c}$-behavior resulting from double exchange, while the LDA+U results are more or less linear in c, indicating that in (Ga, Mn)As the kinetic p-d exchange is most important [13]. This exchange mechanism underlies all model calculations based on the Kondo Hamiltonian, which describe the physics of (Ga, Mn)As rather well. However the physics of the impurity band systems is very different and cannot be described by such a Hamiltonian (although this is very often done).

5 Exchange Coupling Constants and Curie Temperatures

The exchange coupling constants J_{ij} give according to eq. (7) the information about the orientational coupling between the local moments M_i and M_j. For the DMS-systems they have been calculated by embedding the two magnetic impurities i and j in the CPA medium of the ferromagnetic state, in this way including the substitutional disorder of all other impurities in an average way. As a result, the coupling constants are strongly concentration dependent due to the magnetic screening of the other impurities.

The calculated J_{ij} constants for (Ga, Mn)N, (Ga, Mn)P, (Ga, Mn)As and (Ga, Mn)Sb are shown in Fig. 9 for three different concentrations, i.e., 1 %, 5 % and 15 % of Mn impurities. The results show a qualitatively very different behaviour, in particular for the two extreme cases of (Ga, Mn)N and (Ga, Mn)Sb. In (Ga, Mn)N the interaction is very strong for the nearest neighbors, but the coupling of the further away atoms is very small. This is typical for the double exchange mechanism mediated by the impurity band. The coupling arises from the overlap of the impurity states on neighboring sites. Since these states are relatively well localised, the coupling is strong, but short ranged. (Ga, Mn)Sb represents the other extreme, the coupling of which is dominated by p-d exchange. Here the coupling is weak, but very long ranged. This arises from the large spatial extent of the Sb-p states near the valence band maximum, since the interaction is basically transferred by the spin polarised hole states at the Γ point.

The estimation of the Curie temperature T_{C} by the mean field expression $\frac{1}{3}c\sum_{i\neq 0} J_{0i}$ is very problematic for dilute systems with low concentrations, since it does not require any information on the interaction range. This simplification leads to significant errors in the calculations of T_{C} for low concentrations [17, 18]. It can be easily understood and is known as the percolation problem [19]. Let us consider a Heisenberg model with a ferromagnetic exchange interaction only between nearest neighbors (nearest neighbor Heisenberg model), and see what happens when the system is diluted with non-magnetic sites as schematically shown in Fig. 10-(a).

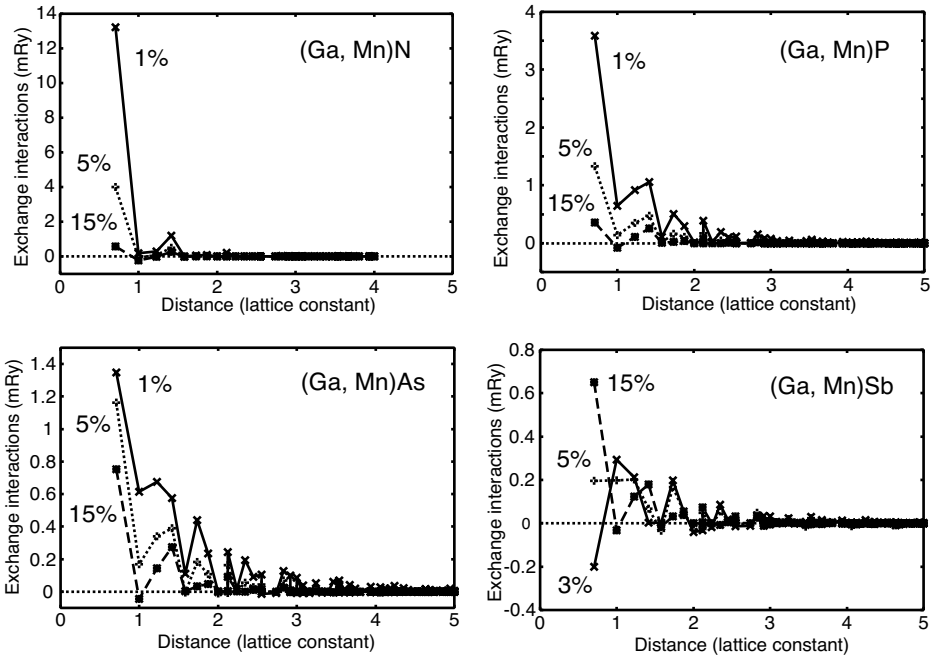

Figure 9: Exchange coupling constants J_{ij} between two Mn atoms as a function of the distance for three different concentrations. The concentration dependence arises from the screening effects of the other impurities, being described by the embedding of the two impurities in the CPA medium.

When the concentration of magnetic sites is 100 % , we have a perfect ferromagnetic network. Due to the dilution, the network is weakened, and for a concentration below a percolation threshold the ferromagnetism cannot spread all over the system leading to paramagnetic state since due to missing longer ranged interactions the moments can no longer align. Obviously this effect is not counted in the mean field equation for T_{C}, because the dilution effect is included only as a concentration factor c in the equation. In case of the nearest neighbor Heisenberg model, the percolation threshold c_p for the fcc structure is 20 % (note that the impurities sit on the fcc Ga sublattice of the zinc blende structure). In real systems such as (Ga, Mn)N the interaction reaches beyond the nearest neighbors and the real percolation threshold should be lower. However, below 20 % the strong nn coupling is not so important anymore, since only the much weaker longer ranged interaction induces the ferromagnetism, so that the Curie temperature is expected to drop considerably and to be much smaller than the mean field value, being determined to a large extent by the strong nn coupling J_{01}.

In order to take the percolation effect into account, we perform Monte Carlo simulation (MCS) for the classical Heisenberg model. The thermal average of magnetization M and its powers are calculated by means of the Metropolis algorithm [20]. Due to the finite size of super cells used in the simulation, it is difficult to determine T_{C} from the temperature dependence of $\langle M(T)\rangle$. In particular, when considering dilute systems, finite size effects and appropriate finite size scaling are of particular importance for a correct and efficient evaluation of T_{C} by Monte Carlo simulations. To avoid this difficulty, we use the cumulant crossing method proposed by Binder [20]. This method uses the finite size scaling in the forth order cumulant U_4 which is defined as $U_4 = 1 - \langle M^4\rangle/(\langle M^2\rangle)^2$. U_4 is calculated for various cell sizes and plotted as a function of

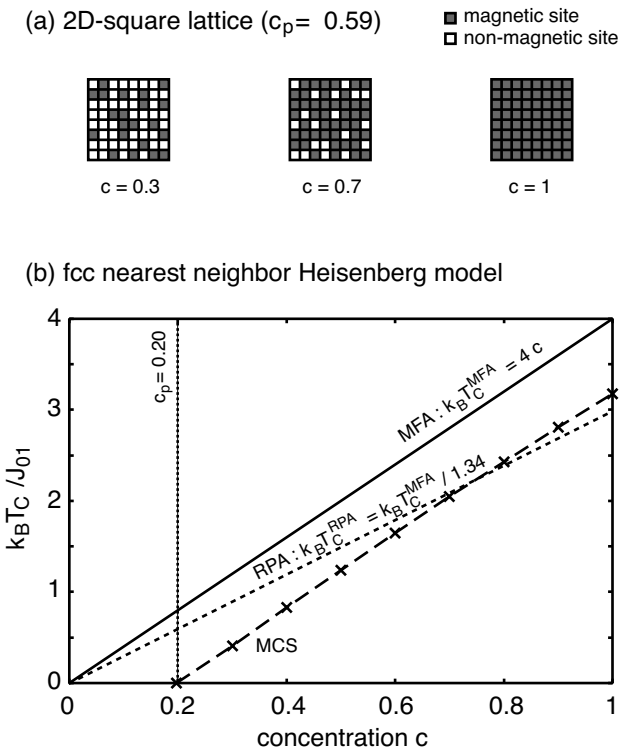

Figure 10: (a) Schematic picture of dilute 2-dimensional nearest neighgor Ising model in square lattice. The percolation thereshold is 0.59 in this case. (b) Curie temperatures of the classical nearest neighbour Heisenberg model for the fcc lattice as a function of the concentration. The full line gives the mean field results, being linear in c. The crosses connected by the dashed line give the exact values as obtained by Monte Carlo simulations (MCS), which vanish below the percolation threshold of $c_p = 20$ %. The nn coupling constant J_{01} has been fixed at a constant value.

temperature. If the cell size is larger than the correlation length, it can be shown that the $U_4(T)$ curves for different sizes cross each other at three characteristic temperatures. Two of them are $T = 0$ and $T = \infty$, and the other is $T = T_{\rm C}$. We use 3 cell sizes ($6 \times 6 \times 6, 10 \times 10 \times 10$ and $14 \times 14 \times 14$ conventional fcc cells) to carry out the cumulant crossing method for $T_{\rm C}$ calculations.

First, as a pedagogical example we show the calculated $T_{\rm C}$ for the dilute fcc nearest neighbour Heisenberg model as calculated by MFA and MCS in Fig. 10-(b). For MCSs for dilute systems, we take 30 different random configurations of magnetic sites for the ensemble average. As shown in Fig. 10-(b), it is found that the MFA gives a reasonable, but too high estimation of $T_{\rm C}$ for $c = 1$. However, with decreasing c both curves decline with nearly the same slope and below the percolation threshold, $c_p = 0.20$, the Curie temperature vanishes. Thus in the dilute concentration range below 20 %, which is most relevant for DMS systems, the failure of the MFA is evident [17, 18].

Next, we show the calculated $T_{\rm C}$ values of (Ga, Mn)N (Fig. 11-(a)) and (Ga, Mn)As (Fig. 11-(b)) as obtained by the MCS from the J_{ij} values in Fig. 9. Thirty configurations of Mn atoms are considered for averaging and J_{ij} interactions up to 15 shells are included. As shown in Fig. 11-(a), very small $T_{\rm C}$ values are predicted for low concentrations in (Ga, Mn)N. The MFA values are almost 2 orders of magnitude too large. Thus we find that the magnetism is

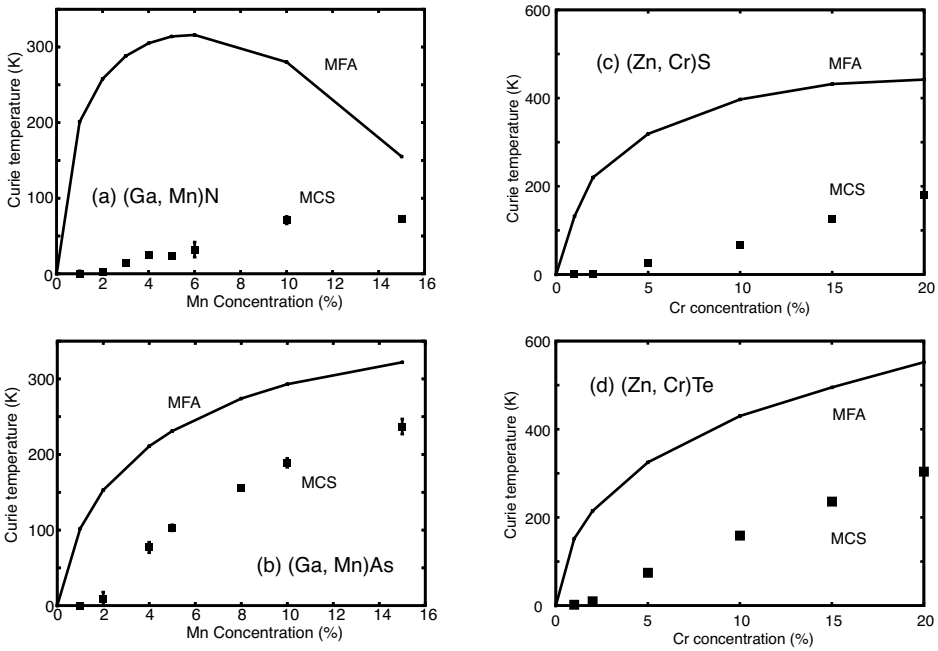

Figure 11: Curie temperatures of (a) (Ga, Mn)N, (b) (Ga, Mn)As, (c) (Zn, Cr)S and (d) (Zn, Cr)Te as evaluated in the mean field approximation (MFA) and by Monte Carlo simulations (MCS) from the J_{ij} values obtained in the LDA (see Fig. 9). Due to the percolation problem the Curie temperature of (Ga, Mn)N is strongly reduced for small concentrations. This effect can also be seen in (Zn, Cr)S and (Zn, Cr)Te. Due to the longer interaction range the reduction of Curie temperatures effect is more moderate in (Ga, Mn)As.

strongly suppressed due to the missing percolation of the strong nearest neighbour interactions. Only the weak, longer ranged interactions satisfy the percolation requirement, leading to small but finite Curie temperatures for 5, 10 and 15 % of Mn. As shown in Fig. 11-(b), due to the longer ranged interaction in (Ga, Mn)As, the reductions from the MFA are not very large, but still significant. Naturally these changes are larger for smaller concentrations. The T_{C} values of 103 K obtained for 5 % Mn is in good agreement with the experimental values of 118 K reported by Edmonds et al. [21]. This values refers to measurements in thin films which are free of Mn-interstitials representing double donors. Including interactions beyond 15th shell, MCS could give slightly higher T_{C} values for low concentrations. At very high concentrations we expect our results to increase towards the MFA values.

The experimental situation for T_{C} in (Ga, Mn)N is very controversial. There are many reports, where very high Curie temperatures, well above room temperature, have been observed, but also many observations of no ferromagnetism or only very low Curie temperatures. The above calculations suggest, that a homogeneously ferromagnetic phase with a Curie temperature around or above room temperature can be excluded. Therefore the experimentally observed very high T_{C} values have to be attributed to small ferromagnetic MnN clusters and segregated MnN phases, where the strong ferromagnetic nn interaction becomes fully effective.

The same method for calculating T_{C} is applied to (Zn, Cr)S and (Zn, Cr)Te as typical examples of II-VI DMS systems [22]. Results are shown in Fig. 11-(c) and -(d). In these compounds, impurity t-bands appear in the gap and 2/3 of the impurity bands are occupied (namely, they

are equivalent to Mn-doped III-V DMS such as (Ga, Mn)N from electron occupation point of view), therefore the double exchange is dominant mechanism. As a result, MFA values of T_C show $\sqrt{c}$ dependence. For both cases, MCS values of T_C deviate very much from MFA values due to the same reason in the case of (Ga, Mn)N. The suppression of the ferromagnetism in (Zn, Cr)S at small concentrations is as significant as in (Ga, Mn)N. The effect is slightly moderate in (Zn, Cr)Te than in (Zn, Cr)S, because ZnTe has smaller band gap than ZnS and the Cr t-band is very near to the host valence band in (Zn, Cr)Te [22]. Calculated exchange interactions of (Zn, Cr)Te are short ranged but not as short as in (Ga, Mn)N. The observation of a T_C value of 300 K for (Zn, Cr)Te with 20 % Cr is in good agreement with MCS results. The linear scaling in MCS values of T_C in Fig. 11-(d) has been observed in recent experiments [23, 24]

6 Summary

Due to their half-metallicity and structural similarity to semiconductors dilute magnetic semiconductors are hopeful materials for a future spintronics. However the Curie temperatures are in general very low. In this review we have discussed the origin of ferromagnetism in these materials and presented ab-initio calculations for the electronic and magnetic properties of (Ga, Mn)N, (Ga, Mn)P, (Ga, Mn)As and (Ga, Mn)Sb. The results point of the existence of two classes of DMS with very different properties:

(i) In systems with localised majority d-states deep in the valence band such as (Ga, Mn)As and (Ga, Mn)Sb, the ferromagnetism is induced by Zener's p-d exchange, leading to holes in the majority p-valence band. This interaction is relatively weak, but long ranged. At small concentrations the Curie temperature is only moderately reduced by the percolation effect.

(ii) In systems with impurity-bands in the band gap such as (Ga, Mn)N and (Zn, Cr)Te, the ferromagnetism is driven by Zener's double exchange. Here the magnetic coupling is strong, but short ranged. Therefore, in the dilute limit the ferromagnetism is strongly suppressed, since percolation of the strong nearest neighbor interactions cannot be achieved.

A way to achieve higher Curie temperatures might be to try to increase the impurity concentration. For the p-d systems this should help, since the Curie temperature basically scales linearly with the concentration. For the impurity band systems the percolation effects become less important at higher concentrations, so also here higher concentrations would help. The observation of the T_C of 300 K for 20 % Cr doped ZnTe supports this argument [23, 24].

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