### PROGRAMME RTN COMPUTATIONAL MAGNETOELECTRONICS

**2nd Annual Meeting and Mid-Term Review**  
**Oleron Island, October 5-9, 2002**

**Saturday October 5**

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<td>15:40 - 16:20</td>
<td>Theoretical aspects of spin-dependent tunneling. <em>(Juergen Henk)</em></td>
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<td>16:20 - 17:00</td>
<td>Coffee</td>
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<td>17:00 - 17:40</td>
<td>The role of transverse spin accumulation in current induced switching of magnetization <em>(Peter Levy)</em></td>
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<td>17:40 - 18:20</td>
<td>Ferromagnet/Semiconductor interfaces <em>(Susanne Mirbt)</em></td>
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<td>19:15 - 20:15</td>
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**Poster Session 1:**  
**Saturday October 5 - 6**

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<td>P02</td>
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<td>A.L. Klavsyuk</td>
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<td>P03</td>
<td>Spin motion in electron transmission through ultrathin ferromagnetic films</td>
<td>Juergen Henk</td>
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<td>P04</td>
<td>Beyond LDA: GW and SIC implementation in KKR</td>
<td>Arthur Ernst</td>
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<td>P05</td>
<td>Quantum-size effects in ultrathin Ag films on V(001): Electronic structure and photoelectron spectroscopy</td>
<td>Arthur Ernst</td>
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<td>P06</td>
<td>Electronic structure and tunnel magnetoresistance of Fe/MgO/Fe</td>
<td>M. Bouhassoune</td>
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<td>P07</td>
<td>In-plane uniaxial anisotropy at the Fe/ZnSe(001) interface</td>
<td>Lars Nordstrom</td>
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<td>P08</td>
<td>An embedded Green-function approach to ballistic electron transport through an interface</td>
<td>D. Wortmann</td>
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<td>P09</td>
<td>Ballistic Spin Injection from Fe into ZnSe and GaAs</td>
<td>O. Wunnicke</td>
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<td>P10</td>
<td>Ab initio investigations of Fe/W(110): Magnetic Structure of Domain-Walls</td>
<td>M. Heide</td>
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<td>P11</td>
<td>Surface core level shift used as a tool to identify PdMn systems on Pd(100)</td>
<td>W. Olovsson</td>
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<td>P12</td>
<td>Multiple-scattering theoretical approach to scanning tunneling spectroscopy</td>
<td>P. Karas</td>
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<td>P13</td>
<td>Half-ferromagnetism and Slater-Pauling behavior in the Heusler alloys</td>
<td>I. Galanakis</td>
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<td>P14</td>
<td>Electronic and magnetic properties of ferromagnet/semiconductor interfaces</td>
<td>M. Kosuth</td>
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<td>P15</td>
<td>Relativistic effects in the transport properties of FM/SC/FM trilayer systems</td>
<td>V. Popescu</td>
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<td>P16</td>
<td>Probing magnetic susceptibilities using the field-induced magnetic circular dichroism</td>
<td>S. Mankovsky</td>
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<td>P17</td>
<td>Disorder-induced magnetism in TiFe$<em>x$Co$</em>{1-x}$ (D. Benea)</td>
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<td>P18</td>
<td>LMTO Green Function approach for the ab initio calculation of the optical and magneto-optical properties of solids (S. Chadow)</td>
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<td>P19</td>
<td>Electron-electron interaction viewed by one-photon two-electron excitations (J. Berakdar)</td>
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<td>P20</td>
<td>Magnetization of the unsegregated and segregayed (100) surface of MoV binary alloy (L.V. Pourovskii)</td>
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<td>P21</td>
<td>First-principle study of the magnetoresistance effects in magnetic nanocontacts (A. Bagrets)</td>
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<td>P22</td>
<td>Phase separation at interfaces in La$<em>{2/3}$Ca$</em>{1/3}$MnO$_3$ (M. Bibes)</td>
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<td>P23</td>
<td>Magnetic nanostructures on metal surfaces (V.S. Stepanyuk)</td>
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<td>P24</td>
<td>The influence of hydrogen adsorption on magnetic properties of Ni/Cu(100) surface (F. Maca)</td>
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<td>P25</td>
<td>Giant Magnetoresistance in carbon nanotubes (S.P. Athanasopoulos)</td>
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<td>P26</td>
<td>Relativistic calculation of spin-wave spectra in thin magnetic films (L. Udvardi)</td>
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<td>P27</td>
<td>Exchange interactions in magnetically frustrated systems (I.A. Abrikosov)</td>
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<tr>
<td>9:00</td>
<td>Spin-polarized diffusive transport in ferromagnetic metal/semiconductor heterostructures (Albert Fert)</td>
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<tr>
<td>9:40</td>
<td>Proximity Effects Between Superconductors and Ferromagnets (Balazs Gyorffy)</td>
</tr>
<tr>
<td>10:20</td>
<td>Coffee</td>
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<tr>
<td>11:00</td>
<td>First-principles theory of semiclassical spin and charge transport (Paul J. Kelly)</td>
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<tr>
<td>11:40</td>
<td>Ab initio characterization of the giant magnetoresistance in realistic spin valves (Laszlo Szunyogh)</td>
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<tr>
<td>12:30</td>
<td>Lunch</td>
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<tr>
<td>14:00</td>
<td>Social Event</td>
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<tr>
<td>19:00</td>
<td>Dinner</td>
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<td>20:30</td>
<td>Posters 2</td>
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<th>Time</th>
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<tr>
<td>9:00</td>
<td>Exchange interactions in bulk and layered itinerant magnets (Ilja Turek)</td>
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<tr>
<td>9:40</td>
<td>Half metallic transition metal oxides (Dzidka Szotek)</td>
</tr>
<tr>
<td>10:30</td>
<td>Coffee</td>
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<tr>
<td>11:00</td>
<td>Fundamental tunneling studies using the half-metallic manganite La$<em>{0.7}$Sr$</em>{0.3}$MnO$_3$ (Martin Bowen)</td>
</tr>
<tr>
<td>11:40</td>
<td>Magnetic and transport properties of ferromagnet/semiconductor/ferromagnet systems (H. Ebert)</td>
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<tr>
<td>12:30</td>
<td>Lunch</td>
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<tr>
<td>14:00</td>
<td>Study of half-metallicity in LSMO junctions (G. Banach)</td>
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<td>14:30</td>
<td>Andreev Bound States and Spontaneous Currents in Ferromagnet -Superconductor Heterostructures (M. Krawiec)</td>
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<tr>
<td>15:00</td>
<td>CPP-transport calculations in Co/Cu (001) and (111) trilayers. (O. Bengone)</td>
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<tr>
<td>15:30</td>
<td>Spin-injection through an Fe/InAs Interfaces (M. Zwierzycki)</td>
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<td>Time</td>
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<tr>
<td>16:00</td>
<td>Coffee</td>
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<tr>
<td>16:30</td>
<td>Perpendicular electric transport in Fe/Si/Fe trilayers: influence of alloying and interdiffusion (H. Herper)</td>
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<tr>
<td>17:00</td>
<td>Towards New Half-Metallic Systems: Zinc-Blende Compounds of Transition Elements with N, P, As, Sb, S, Se and Te (P. Mavropoulos)</td>
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<td>17:30</td>
<td>(P. Vlaic)</td>
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<td>18:00</td>
<td>Quantitative theory of the Invar anomaly in RECo2 and magnetization processes in Y(Co1-xAlx)2 compounds (S. Khmelevskyi)</td>
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<tr>
<td>18:30</td>
<td>Multiple-scattering theoretical approach to scanning tunneling spectroscopy (P. Karas)</td>
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<tr>
<td>18:40</td>
<td>Bandgap dependence of the interlayer exchange coupling (T. Dziekan)</td>
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<td>19:00</td>
<td>Conference Dinner</td>
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<td>20:30</td>
<td>6th Framework Talk</td>
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<td>21:30</td>
<td>Open Network Management Meeting</td>
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<tr>
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<td>Mid-Term Review</td>
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<tr>
<td>10:15</td>
<td>Coffee</td>
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<tr>
<td>10:45</td>
<td>Mid-Term Review</td>
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<tr>
<td>12:00</td>
<td>Lunch</td>
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<tr>
<td>15:00</td>
<td>Symposium on Magnetic Semiconductors and Half-Metallic Systems</td>
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<tr>
<td>15:40</td>
<td>Control of spin ordering in ferromagnetic semiconductors (Tomasz Dietl)</td>
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<td>16:00</td>
<td>Coffee</td>
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<tr>
<td>17:00</td>
<td>On the electronic state of Mn impurities in GaAs (Thomas Schulthess)</td>
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<td>17:40</td>
<td>Tunnel magnetoresistance of epitaxial double barrier tunnel junctions based on the ferromagnetic semiconductor GaMnAs (Richard Mattana)</td>
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<td>18:05</td>
<td>Electronic and magnetic structure of Cr and Mn doped GaAs (Olle Eriksson)</td>
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<td>18:30</td>
<td>Exchange interactions and Curie temperature in (GaMn)As (L. Sandratskii)</td>
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<td>19:15</td>
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<td>9:00</td>
<td>Ab initio study of group IV and III-V magnetic semiconductors (J. Kudrnovsky)</td>
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<tr>
<td>9:25</td>
<td>Phase stability and ordering in (Ga,Mn)As alloys (V. Drchal)</td>
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<td>9:50</td>
<td>Critical temperatures of diluted magnetic semiconductors. (L.Bergqvist)</td>
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<tr>
<td>10:15</td>
<td>Coffee</td>
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<tr>
<td>11:10</td>
<td>Magnetism in diluted magnetic semiconductors (B. Sanyal)</td>
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<tr>
<td>11:35</td>
<td>Electronic structure and Curie temperatures of diluted magnetic semiconductors (K. Sato)</td>
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<td>12:00</td>
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2nd Annual Meeting and Mid-Term Review

Oleron Island, October 5-9, 2002

LECTURES
Spin-filter effects in metallic nanowires and nanocontacts

N.Papanikolaou\textsuperscript{a}, A.Bagrets\textsuperscript{b}, J.Opitz\textsuperscript{a}, P.Zahn\textsuperscript{c} and I.Mertig\textsuperscript{a}

\textsuperscript{a} Martin-Luther-Universität Halle, Fachbereich Physik, D-06099 Halle, Germany
\textsuperscript{b} Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany
\textsuperscript{c} Uppsala Universitet, Fysika Institutionen, SE-75121 Uppsala, Sweden

We present ab-initio calculations of electronic transport in metallic nanowires and nanocontacts. We consider translationally invariant wires with a diameter of few atoms. The nanocontacts are modeled by short chains of atoms embedded between semi-infinite leads. We used a first-principle screened Korringa-Kohn-Rostoker Green’s function method to calculate the electronic structure of the nanowires and nanocontacts. The electronic transport properties were obtained using the Landauer formalism. We have investigated the effect of transition metal impurities on the conductance of the nanowires and nanocontacts. We will demonstrate that single impurities can easily block the conducting channels in nanowires and reduce the conductance. Impurity pairs however cause quantum interference effects and give rise to a complicated energy dependence of the conductance. In nanocontacts we will show how the spin is transmitted through atomic chains and how nanocontacts can act as spinelectronic devices.

Theoretical aspects of spin-dependent tunneling

J. Henk and P. Bruno

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

The idea to exploit the electron spin in electronic circuits (spintronic) has lead to a vast amount of both experimental and theoretical work. However, even simple systems—like tunnel junctions which consist of two ferromagnetic electrodes separated by a nonmagnetic spacer—are challenging theory and provide new insights. In this topical review, I shall discuss some theoretical aspects of spin-dependent tunneling.

The first part of the talk is concerned with planar tunnel junctions. Regarded as a scattering process, tunneling can naturally be formulated within multiple-scattering theory (e.g., layer-KKR). Starting from \textit{ab-initio} calculations (DFT, LSDA), the tunneling conductances are obtained from Landauer-Büttiker theory. Besides technical details — like efficient Brillouin zone integration — I shall discuss ‘hot spots’ in the tunneling transmission of Ni/Vacuum/Ni and the importance of the interface structure for Fe/MgO/Fe. The dependence of the tunnelmagnetoresistance on the bias voltage is addressed for Co/Vacuum/Co.

The second part focuses on scanning tunneling spectroscopy. Formulating the tunneling process within scattering theory provides a straight-forward implementation in multiple-scattering theory which goes beyond the popular Tersoff-Hamann approach. Model calculations reveal the power of this ansatz.
A self-consistent treatment of non-equilibrium spin torques in magnetic multilayers

Peter M. Levy

The concept of using a spin polarized current to switch the orientation of a magnetic layer was developed by Slonczewski and Berger, and has been followed up by others. Recently, we have proposed a way to understand this spin transfer torque by adopting the model we used to understand magnetoresistance for currents perpendicular to the plane of the layer (CPP), namely, two phenomena, CPP magnetoresistance (MR) and spin torque, originate from the spin accumulation. The former is primarily associated with the longitudinal spin accumulation and the latter is governed by a transverse effect. The distinguishing feature between previous treatments and the one we recently outlined lies in our focus on the spin transport for the entire CPP structure rather than for the interface region alone, i.e., we consider the spin torque due to the bulk of the magnetic layers and the diffuse scattering at interfaces.

Among the points I plan to highlight in my presentation are that the angular momentum transferred to a thin layer, that is to be switched, far exceeds the transverse component (to the orientation of the magnetization of the thin layer) of the bare portion of the incoming spin polarized current, i.e., that part proportional to the electric field. This is a direct consequence of the spin accumulation coming from the two primary layers, the thick magnetic and nonmagnetic back layers, that produce this buildup. The role of this accumulation in the spin current is a consequence of considering the transport in the multilayer as a diffusive process, and is in keeping with previous treatments of transport in magnetic multilayers. Among other things the parameters entering our theory are determined from CPP transport measurements, except for the exchange interaction between the itinerant electrons and the magnetic background. I will show why this exchange constant is smaller than what can be inferred from LSDA band structure calculations.
Ferromagnet/Semiconductor interfaces

Susanne Mirbt

We have studied the structural and magnetic properties of Fe on GaAs(100) and ZnSe(100). Calculations involving full geometry optimizations have been carried out for a broad range of thickness of Fe layers (0.5-10 ML) on top of both a GaAs and ZnSe substrate. Both cation and anion terminated interfaces have been explored. Total energy calculations show that the anion segregates at the surface in agreement with experiment.

Spin polarized transport in ferromagnetic metal/semiconductor heterostructures

A. Fert and H. Jaffrs

Unit Mixte de Physique CNRS-Thals, Domaine de Corbeville, 91404 Orsay, France, and Universit Paris-Sud, 91405 Orsay, France.

Tunnel barriers or Schottky contacts at the interface between a ferromagnetic metal and a semiconductor can present interesting spin filtering properties, as this is shown in several communications at this meeting. However having a spin dependent transmission through the interface is not the only condition and, even with a spin dependent tunnel or Shottky junction, the injected current can be non-polarized. This comes from the unbalance between the spin accumulation and relaxation effects in the two materials. This unbalance problem led Schmidt et al [1], a few years ago, to conclude that a spin polarized current cannot be injected from a metal into a semiconductor. In our presentation at OIron, we will show how one can get round the fundamental difficulty raised by Schmidt et al, and how an efficient spin injection can be achieved. We also discuss the problem of spin transmission and spin detection in several types of ferromagnetic metal/semiconductor heterostructures. By adapting the spin accumulation model of the perpendicular transport in metallic magnetic multilayers to the situation of ferromagnetic metal (F)/semiconductor (SC) heterostructures [2], we show that the problem of spin injection between F and SC can be solved by introducing a well-adapted spin dependent interface resistance (tunnel junction preferably) at the F/SC interfaces. In the little more complex situation of a F/SC/F structure, a significant value of the magnetoresistance (signature of spin injection + electrical spin detection) can be obtained if the junction resistance is chosen between two threshold values depending on the resistivity, spin diffusion length and thickness of SC. We illustrate the results of our model with numerical calculations for Co/GaAs/Co structures. Our results on F/SC/N structures are at odds with recent theoretical results of Rashba [3] and we explain the origin of the discrepancy. Finally we will present extensions of our approach to other types of geometry (injection into a 2DEG, double tunnel junctions, etc). We will also discuss interesting effects expected for high current densities.

Proximity Effects Between Superconductors and Ferromagnets

Balazs L. Gyorgy
University of Bristol

As has been discovered in the 1960-ies a superconductor in contact with a normal metal can induce pairing correlations in the latter. Although this, surprising, Proximity Effect is by now well understood a version of it which occurs when the normal metal is ferromagnetic is attracting current interest. I shall review the recent advances in our understanding of the Proximity Effect in such hetero structures and argue that they are of both scientific and technological interest. In particular I will emphasis the unique role they can play in the study of interaction between magnetism and superconductivity and comment on their significance in the context of spin-dependent transport.

First-principles theory of semiclassical spin and charge transport

Paul J. Kelly

Spin and charge transport in the semiclassical regime is governed by the scattering matrices of interfaces which connect the distribution functions in the bulk materials on either side. We review the results of first-principles calculations of the scattering matrix as applied to various physical properties like spin-dependent interface resistances, Andreev scattering, spin current-induced magnetization torque, angular magnetoresistance, Gilbert damping of magnetization dynamics and spin-injection into semiconductors. We emphasize the importance of interface disorder and the phase of the elements of the scattering matrix and, where available, compare theoretical results with experiments.

Ab initio characterization of the giant magnetoresistance in realistic spin valves

P. Weinberger
Technical University of Vienna, Austria
L. Szunyogh
Budapest University of Technology, Hungary
The electric transport properties of a rather complicated spin valve system containing NiFe permalloy, CoFe hard magnets and two types of spacers (Cu,Ru) are investigated theoretically in terms of the of the Screened Korringa-Kohn-Rostoker method and the Kubo-Greenwood equation. It is found that the regimes of antiferromagnetic coupling are mostly determined by the thickness of the Cu spacer: the nodes of oscillation of the interlayer exchange coupling (IEC) with respect to the Cu spacer thickness are shifted only marginally by the presence of a very thin Ru spacer. The oscillations of the IEC and the giant magnetoresistance (GMR) are investigated with respect to the thickness of the hard magnet parts of the system (CoFe). The minima viewed with respect to the thickness of the Cu spacer and also the actual values of the GMR are in reasonable agreement with experiment.

Exchange interactions in bulk and layered itinerant magnets

I. Turek


J. Kudrnovský, V. Drchal

Institute of Physics, Acad. Sci. Czech Rep., Prague

P. Bruno

MPI für Mikrostrukturphysik, Halle, Germany

S. Blügel

Institut für Festkörperforschung, FZ Jülich, Germany

The talk reviews a two-step procedure to determine thermodynamic properties of itinerant magnets from first principles. In the first step, the selfconsistent electronic structure of a system is calculated using the tight-binding linear muffin-tin orbital method combined with Green function techniques, which is appropriate for description of substitutional randomness of disordered bulk alloys and for two-dimensional translational periodicity of layered systems like surfaces and thin films. In the second step, the parameters of the effective classical Heisenberg Hamiltonian are determined using the magnetic force theorem and they are employed in subsequent evaluation of magnon spectra, the spin-wave stiffness constants and critical temperatures. Examples of application include: (i) ferromagnetic 3d metals Fe, Co, and Ni, (ii) disordered binary transition-metal alloys, (iii) ultrathin magnetic films of Fe and Co on a Cu(001) substrate, (iv) diluted magnetic semiconductors (Ga,Mn)As, and (v) 4f electron systems like hcp Gd and bcc Eu. The developed theory will be presented together with selected aspects of the numerical implementation and with a comparison to existing experimental data.

Half-metallic transition metal oxides

Z. Szotek

Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK

In this talk we briefly overview the characteristics and applications of half-metallic ferromagnets. We discuss an application of the self-interaction corrected
local spin density approximation (SIC-LSD) to some half-metallic compounds, and among them the double perovskites $\text{Ba}_2\text{FeMoO}_6$, $\text{Ca}_2\text{FeMoO}_6$, $\text{Sr}_2\text{FeMoO}_6$, $\text{Ca}_2\text{FeReO}_6$, and magnetite ($\text{Fe}_3\text{O}_4$). We also mention briefly mixed valence manganite compounds, and show that also such simple transition metal monoxides as NiO and MnO can show half-metallic characteristics when doped with vacancies. In the double perovskites we concentrate on the electronic and magnetic properties of these compounds and in particular the size and relative orientation of the spin moments of Fe and Mo or Re. In all the compounds the calculations find a spin moment of about 0.4 $\mu_B$ on the Mo sites and $\sim 1.0$ $\mu_B$ on Re, with an opposite orientation to the respective spin moments on Fe sites. We find these double perovskites to be half-metallic, with a well defined gap in the spin-up density of states, and strong hybridization at the Fermi energy between the spin-down Fe 3$d$, Mo 4$d$ (or Re 5$d$), and O 2$p$ states. Issues of charge ordering in magnetite are also discussed. We find that the charge ordered phase is not the groundstate solution for this compound.

**Fundamental tunneling studies using the half-metallic manganite $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$**

M. Bowen$^1$, M. Bibes$^1$, R. Bertacco$^2$, A. Barthlmy$^1$, M. Portalupi$^2$, M. Marcon$^2$, L. Duo$^2$, F. Cicacci$^2$, J.P. Contour$^1$, A. Fert$^1$, F. Petroff$^1$, E. Jacquet$^1$, J. Humbert$^1$, A. Vaurs$^1$

(1) *Unit mixte de Physique CNRS/THALES, Domaine de Corbeville, 91404 Orsay Cedex, France, and Universit Paris-Sud, 91405 Orsay Cedex, France*

(2) *INFN Dipartimento di Fisica, Politecnico de Milano, P.za L. da Vinci 32, 20133 Milano, Italia Tel: 33-1-69-33-92-53, Fax: 33-1-69-33-07-40, martin.bowen@thalesgroup.com*

To better understand certain fundamental aspects of tunneling, we have integrated the half-metallic manganite $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (001) (LSMO), grown in an epitaxial bilayer with an insulating barrier of $\text{SrTiO}_3$ (001) (STO), into magnetic tunnel junctions. LSMO/STO/LSMO junctions yield up to 1800 magnetoresistance for a LSMO spin polarization in excess of 95 in the bias dependence of magnetoresistance in agreement with inverse photoemission experiments [2] performed on LSMO//STO(001) and STO(2ML)/LSMO//STO(001). Conductance studies at high magnetic fields point to a departure in tunneling behavior from interfacial 2D to 3D as the result of using junction electrodes with a more delocalized double exchange conduction mechanism rather than the more conventional metallic behavior of transition ferromagnets. Finally, to understand the influence of the epitaxial barrier on tunneling, we will present preliminary transport results on LSMO-based junctions which integrate an epitaxial TiO2 barrier [4].

1 M. Bowen et al. (submitted to App. Phys. Lett.)
2 R. Bertacco, to appear in PRB.
4 M. Bibes et al. (in preparation)
Electronic and magnetic and transport properties of ferromagnet-semiconductor heterostructure systems

H. Ebert, M. Košuth, V. Popescu, A. Perlov, J. Minár, R. Zeller, N. Papanikolaou, and P. H. Dederichs

The electronic and magnetic and transport properties of ferromagnet/semiconductor (FM/SC) heterostructure systems have been studied by means of various band structure methods (LMTO, KKR-CPA, TB-KKR). As a structural model for our calculations periodic multilayer systems as well as half-infinite tri-layer systems have been assumed, taking for the ferromagnet Fe and for the semiconductor GaAs or Ge. Together with the profile of the spin and orbital magnetisation the magneto-crystalline anisotropy has been investigated in detail to check the relationship between the electronic magneto-crystalline anisotropy energy and the anisotropy of the orbital moment as proposed by van der Laan. Making use of the Coherent Potential Approximation (CPA), the influence of interdiffusion at the Fe/GaAs interface within the multilayer system has been studied. On the basis of the electronic structure calculations, the magnetic circular X-ray dichroism (MCXD) has been calculated for the $L_3$-edges absorption spectra of Fe, Ga and As in the near-edge regime (XANES). The transport properties of FM/SC heterostructure systems were studied by making use of a relaxation time approach. The results were combined with data for the exchange coupling to give the conductivity as a function of an external magnetic field. In addition to these model studies first principle calculations of the conductance of FM/SC tri-layer systems have been made using the TB-KKR method in combination with the Landauer Büttiker formalism. Attention has been paid in particular to the influence of the spin-orbit coupling. It turned out the TMR ratio can be reduced in a rather appreciable way by the spin-orbit coupling with the conductance of the anti-ferromagnetic configuration more influenced than the ferromagnetic one.

Study of half-metallicity in LSMO junctions.

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We perform one-electron calculations for $La_{1-x}Sr_xMnO_3$ (LSMO) and SrTiO$_3$ (STO), and for the surfaces of these materials, and also the interface of LSMO/STO. TB-LMTO-LSDA and SIC-LSDA LMTO-ASA methods were used. The calculations for nonstochiometric perovskites were based on a stochiometric supercell model ($[La_2SrMnO_3]_n$, where $n=1, 2, 3$) and a rigid band model. We confirmed earlier results of Picket and Singh [1] for LSMO, a strongly polarised electronic structure, nearly half-metallic was obtained. From SIC-LMTO calculations we found of half-metallic state for LSMO for manganese configuration Mn$^{3+}$, where the localise electrons are the $3t_2g$ and one eg. The supercell method was used to model LSMO and STO surfaces. A first calculation for the junction LSMO/STO/LSMO was accomplished for interface MnO/SrO.

Andreev Bound States and Spontaneous Currents in Ferromagnet - Superconductor Heterostructures

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We discuss the ground state properties of an 'insulator - ferromagnet - superconductor' trilayer on the basis of a Hubbard Model featuring exchange splitting in the ferromagnet and electron - electron attraction in the superconductor. We have solved the spin - polarized Hartree - Fock - Gorkov equations together with the Maxwell’s equation (Ampere’s law) fully self-consistently. We have found that due to proximity effect the FFLO - like state [1,2] is realized in such a heterostructure. It manifests itself in oscillatory behavior of the pairing amplitude in the FM and a spontaneously generated spin - polarized current (and magnetic field) in the ground state of the system [3]. We shall discuss the presence of the Andreev bound states, the position of which can be tuned by exchange splitting, and its relation to the current and the pairing amplitude. Finally we will also mention the spin polarization of the current, which is very sensitive to the band filling.

3 M. Krawiec, B. L. Győrffy, J. F. Annett, preprint cond-mat/0203184
4 M. Krawiec, B. L. Győrffy, J. F. Annett, preprint cond-mat/0207135.

CPP-transport calculations in Co/Cu (001) and (111) trilayers.

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A Kubo-Landauer conductance calculation method in the perpendicular geometry, based on transmission matrix formulation has been adapted and implemented in a TB-LMTO-ASA code for general crystallographic orientations of layers. Disorder effects, such as interdiffusion at the interfaces and impurities in different layers, are treated by means of a two dimensions lateral disordered supercell with random distribution of atoms. The present implementation has been applied to Co/Cu trilayers in the fcc (001) and (111) crystallographic orientations. In case of Cr impurity in CoCr/Cu/Co (111) trilayers, an inverse GMR effect is found depending on the magnetic layer thickness, in accordance with experiment.
Spin-injection through an Fe/InAs Interfaces

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

Perpendicular electric transport in Fe/Si/Fe trilayers: influence of alloying and interdiffusion

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We have investigated the electric transport properties of Fe/Si/Fe trilayers in current perpendicular to the plane (CPP) geometry and the interlayer exchange coupling (IEC) depending on the Si layer thickness. Additional effort has been done by examining the influence of interdiffusion, alloy formation at the interfaces, and homogeneous FeSi spacers on the GMR and IEC, because Fe and Si tend to form CsCl-like alloys. It is known from a number of experiments that Fe/Si trilayers or superlattices show a small GMR effect varying between 0.1 and 2.2%. We have been able to demonstrate that this small values for the GMR are related to the existence of interdiffusion at the Fe-Si interfaces. A 5% interdiffusion is already sufficient to decrease the GMR by 50% and a interdiffusion concentration of 50%
leads to small values of the GMR, which are of the same size as the experimental data. Furthermore, it has been shown that these interdiffusion effects also stabilize the AF interlayer exchange coupling.

The electronic calculations have been performed within the fully relativistic spin-polarized version of the Screened KKR method. The transport properties e.g. the resistances have been determined by using the fully relativistic spin-polarized Kubo-Greenwood equation.

Towards New Half-Metallic Systems: Zinc-Blende Compounds of Transition Elements with N, P, As, Sb , S, Se, and Te

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We have studied zinc-blende compounds of the transition metal elements V, Cr, Mn with the sp elements N, P, As, Sb, S, Se, Te. In the ferromagnetic configuration they all show a tendency towards half-metallic behavior, i.e. a band gap in the minority density of states resulting in 100% spin polarization at \( E_F \). This can be traced back to the bonding-antibonding splitting due to hybridization between the transition element \( d \) \( (t_{2g}) \) states and the sp element \( p \) states, conspiring with the large exchange splitting which pushes up the minority \( d \) states. The total moment \( M \) per unit cell, if the system is half-metallic, is integer and given by the \( M = Z - 8 \), where \( Z \) is the number of valence electrons per unit cell. Also, the sp atoms are found to have an antiparallel local moment with respect to the 3d atoms. The electronic and magnetic properties of all these compounds show strong similarities to the corresponding dilute magnetic semiconductors.

We discuss the trends with varying lattice constant, in view of the possibility to grow these materials epitaxially on various semiconductors. Compression eventually kills half-metallicity, since \( E_F \) finally wanders above the minority gap. However, for compounds involving lighter sp elements half-metallicity is encouragingly more robust; this can be explained in terms of the stronger local moment close to the 3d atoms, resulting in a larger exchange splitting and gap.

Finally, we have examined the behavior of the transition element terminated (001) surfaces. In most cases half metallicity is maintained, and the magnetic moment increases because of the missing neighbours where charge would be transfered. Exceptions are the cases where the surface magnetic moment should exceed 5 \( \mu_B \), for which half metallicity is lost.

Quantitative theory of the Invar anomaly in RECo2 and magnetization processes in \( Y(\text{Co}_{1-x}\text{Al}_x)_2 \) compounds

S.Khmelevskyi
We show that the large negative magnetic contribution to the thermal expansion in DyCo2 and HoCo2 can be understood within the s-d (d-f) model. The Invar anomaly in these compounds appears to be a consequence of the metamagnetic properties of the Co sublattice, treated by ab-initio calculations, and the rare-earth local moments coupled to it. It is found, that all finite temperature dynamics of the Invar effect is exclusively governed by the magnetic excitations of the rare-earth moments. Based on TB-LMTO CPA calculations we discuss a problem, which has been debated in the literature for the recent years, namely the possibility of a metamagnetic transition in Y(Co1-xAlx)2 with x¿0.12. Using the Stoner model, but based on actually calculated DOS of Y(Co1-xAlx)2, we study the high-field magnetisation process in these compounds. The results of our investigation suggest that independent of the choice of the Stoner parameter no metamagnetic phase transition occurs above the critical concentration. It is shown that this conclusion is independent on the actual value of the exchange interaction in the system due to peculiar changes in the shape of the density of states with alloying.

Multiple-scattering theoretical approach to scanning tunneling spectroscopy

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The qualitative and quantitative theoretical description of scanning tunneling spectroscopy (STS) is usually based on the popular Tersoff-Hamann model. By simply relating the tunneling current to the spectral density of the sample, however, relevant properties of the tunneling through the tip-sample system are neglected.

Viewing electronic tunneling as a scattering process, we present a formulation of STS in terms of multiple-scattering theory which takes into account the tip-sample interaction. Further, electronic properties of the constituent systems can be obtained by ab-initio calculations. Besides a presentation of the general formalism and its implementation in a spin-polarised relativistic layer-KKR scheme, we sketch results for prototypical systems, with a focus on features of the scattering-theoretical approach.

Bandgap dependence of the interlayer exchange coupling

Thomas Dziekan

LDA method is widely used in solid state physics. But among other things it reproduces the bandgap of semiconductors like GaAs not accurate enough. LDA+U is one approach to overcome this problem. After a short motivation for the choice of the fitting parameter U in GaAs, LDA+U is applied on the Fe—GaAs—Fe multilayer system. We find an increased interlayer exchange coupling with increased bandgap.
Control of spin ordering in ferromagnetic semiconductors

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Recent advances [1] in the field 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 [1,2], will be compared to the case of II-VI compounds, in which the Curie temperatures TC above 1 K have been observed for the uniformly [3] and modulation-doped p-type structures [4] but not in the case of n-type films. The experiments demonstrating the tunability of TC by light [4] and electric field [4,5] will be presented. The tailoring of domain structures and magnetic anisotropy by strain engineering [2,6] and confinement [4] will be discussed emphasizing the role of the spin-orbit coupling in the valence band. The question of designing modulated magnetic structures in low dimensional semiconductor systems will be addressed. Recent progress in search for semiconductors with TC above room temperature and hopes associated with materials containing magnetic ions other than Mn will be presented [1,2].


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Materials Design of New-Class of Diluted Magnetic Semiconductors by ab initio Electronic Structure Calculation: 4f Rare Earth Metal Doping and 3d Transition Metal Doping

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I will discuss the materials design of new-class of diluted magnetic semiconductors based upon ab initio electronic structure calculations. Rare-earth ions doped in semiconductors have been very interesting and attractive for applications to fiber communications as well as medical sensing and surgery. We have succeeded in predicting a new-class of half-metallic ferromagnetic semiconductors doped by rare-earth ions to various wide-band gap III-V semiconductors such as AlN and GaN, which result in drastic enhancement of ferromagnetism due to intra-4f shell of rare-earth ions in the impurity bands. Based upon the total energy calculation between the ferromagnetic states and spin glass states, we have designed the following new-class of ferromagnetic semiconductors. (i) Ce-, Pr-, Nd-, Pm-, Sm-, Eu, Ho- Er-doped GaN and AlN show the half-metallic ferromagnetism. Ce- (5%) doped AlN and GaN show $T_c$ up to 500K without any doping treatment. Gd-doped GaN and AlN is spin glass state, however, electron doping stabilized half-metallic ferromagnetism. (ii) Ce-doped silicon shows the very high Curie temperature ($T_c$) up to 6000K.

We also designed the ferromagnetic semiconductors in 3d transition atom doped IV semiconductors such as diamond (C), silicon (Si) and germanium (Ge). Based upon the total energy calculation between the ferromagnetic states and spin glass states, we have designed the following new class of ferromagnetic IV-th semiconductors. (iii) 3d transition atom doped diamond never show the ferromagnetism because of the strong delocalization of valence and impurity band caused by the too strong p-d hybridization (small lattice constant). (iv) Substitutional Mn-, Fe-, and Co-doped Ge and Si show the ferromagnetism, however, Co-doped Ge is low-spin ground state. Fe-doped Ge and Si is the most stable ferromagnet with high-$T_c$. (v) Interstitial 3d transition metal doped Ge and Si never show the ferromagnetism because of the delocalization of t2 and e-states due to the strong p-d hybridization.

I will discuss the mechanism of high-$T_c$ in the above new systems based upon the competition between the p-d exchange interaction and double exchange interaction. We concluded that the high-$T_c$ is realized based upon the double exchange mechanism, in which stabilization energy caused by the partially occupied itinerant 4f and 3d impurity band dominate the ferromagnetism with high-$T_c$. Low-$T_c$ may be caused by p-d (p-f) exchange interaction.

On the electronic state of Mn impurities in GaAs

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Most phenomenological models of ferromagnetism in Mn doped GaAs assume that the Mn2+ impurity substitutes primarily the Ga3+ cation with five occupied
majority d orbitals that have atomic character and a delocalized acceptor state. While these assumptions are generally thought to be in agreement with experiment, they are presently not supported by ab initio electronic structure calculations. The latter, which are typically based on the Local Spin Density Approximation (LSDA) to Density Functional Theory, find the Mn d orbitals to be strongly hybridized with the As p states. In this picture only four Mn d states are filled with an acceptor state that is localized to the Mn impurity and the first As neighbor shell. It is well known that due to spurious self-interactions LSDA calculations tend to overestimate the hybridization of such impurity states. In the present work we have performed first principles electronic structure calculations of Mn impurities in a GaAs host using the Self Interaction Corrected Local Spin Density Method (SIC-LSD). The method is self interaction free by construction and reproduces the LSDA in the limit of delocalized states. For GaMn-As we find that the self interaction corrections strongly affect the electronic state of Mn. The majority d orbitals are no longer hybridized and are all occupied leaving Mn nominally with S=5/2. The nature of the acceptor states changes as well, in that they have mainly p character and are no longer localized to the Mn site and its nearest neighbors.

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Tunnel magnetoresistance of epitaxial double barrier tunnel junctions based on the ferromagnetic semiconductor GaMnAs

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For spin injection into semiconductors, magnetic semiconductors are an alternative to ferromagnetic metals, with the advantage that the difficulties resulting from the conductivity mismatch between metals and semiconductors can be avoided. On the other hand, magnetic tunnel junctions with magnetic semiconductor electrodes can be used to test spin injection since the existence of tunnel magnetoresistance (TMR) is a signature of the transmission of spin-polarized carriers between the electrodes [1]. We have fabricated single and double barrier magnetic tunnel junctions with GaMnAs electrodes by a low temperature molecular beam epitaxy procedure. The two magnetic electrodes (Ga1-xMnxAs) are separated by a thin AlAs (17) tunnel barrier (single barrier MTJ) or by a AlAs(17)/GaAs(50)/AlAs(17) trilayer (double barrier MTJ). Antiparallel arrangement of the ferromagnetic electrodes at low field is obtained by varying the thickness and Mn concentration in the GaMnAs layers in order to obtain different coercive fields. GaAs layers have been inserted between the electrodes and tunnel barrier in order to avoid the diffusion of Mn into
the tunnel barrier. We observe large TMR effects, progressive saturation of the electrode magnetisation. The existence of similar large MR ratios in the double junction is a new and interesting effect, never observed in metallic double junctions when the intermediate electrode is nonmagnetic. This can be ascribed to the non-relaxed spin splitting of the chemical potential predicted for an intermediate semiconductor electrode [2].


Electronic and magnetic structure of Cr and Mn doped GaAs

O. Eriksson

The electronic structure and magnetic properties of Mn and Cr doped GaAs are reviewed. The effect of lattice relaxation on the magnetic properties are described [1] as well as the effect of lattice impurities[2]. Theoretical values of magnetic moments and critical temperatures are compared to experimental data and avenues for improving the magnetic properties are discussed. In addition phase stability of the Mn-GaAs and Cr-GaAs systems are discussed both for the ideal, defect free case, as well as for the case with As antisite defects[3].

1. B.Sanyal at al. (unpublished)
3. L.Bergqvist et al. (unpublished)

Exchange interactions and Curie temperature in (GaMn)As

L. Sandratskii and P. Bruno

We use supercell and frozen-magnon approaches to study the dependence of the magnetic interactions in (Ga,Mn)As on the Mn concentration. We report the parameters of the exchange interaction between Mn spins and the approximations. In agreement with experiment we obtain a nonmonotonous dependence of the Curie temperature on the Mn concentration. We estimate the dependence of the Curie temperature on the concentration of the carries in the system and show that the decrease of the number of holes in the valence band leads to fast decrease of the Curie temperature. We show that the hole states of the valence band are more efficient in mediating the exchange interaction between Mn spins than the electron states of the conduction band.
The electronic structure of diluted GeMn and (Ga,Mn)As magnetic semiconductors is studied from first principles with a particular emphasis on the effect of various kinds of defects. We map total energies associated with rotations of the Mn-magnetic moments onto an effective Heisenberg Hamiltonian which is then treated in the mean-field approximation in order to find the Curie temperature. The presence of donors like e.g. As-antisites in GaMnAs strongly reduces the Curie temperature. The Heisenberg exchange interactions are reduced with increasing concentrations of both Mn and As in GaMnAs and with increasing concentrations of Mn in GeMn. Calculations indicate an increase of the donor concentration with the increase of the Mn-content in GaMnAs. Finally, we have also investigated the effect of electron correlations included in the framework of the LDA+U method on the properties of GaMnAs alloys.

The phase stability and the possible ordering in ferromagnetic semiconducting alloys is studied from first principles. We determine first the total energies of disordered alloys as a function of their chemical composition. In a next step, by using the generalized perturbation method, we evaluate effective interatomic interactions between impurities by taking into account also the electrostatic interactions. Finally, by employing the methods of statistical physics, namely, by using the linearized version of the concentration wave method we determine the ordering temperature and the k-vector of the transition from the disordered to the ordered state. For temperatures above the ordering temperature we finally calculate the Warren-Cowley short-range order parameters which yield information about the spatial correlation of impurities. As an illustration, we present results for (Ga,Mn)As alloys.
Critical temperatures of diluted magnetic semiconductors.

Lars Bergqvist

Abstract: We have systematically calculated critical temperatures of several diluted magnetic semiconductor systems doped with manganese using supercell and frozen-magnon approaches. By fitting the spin wave energies, using the force theorem, to a Heisenberg expression for magnetic ordering, we have extracted the exchange interactions between the Mn ions. The critical temperatures have been estimated from Monte Carlo simulations and in the few cases where they could be compared with earlier calculations, we find that our approach usually give values between the critical temperatures estimated from mean field and random phase approximations.

Magnetism in diluted magnetic semiconductors

B. Sanyal

Diluted magnetic semiconductors (DMS) are crucial ingredients in magnetoelectronics and semiconductor technology. III-V semiconductors doped with 3d transition metals especially Mn, are the mostly studied materials nowadays. We will present ab-initio electronic structure calculations of transition metal doped semiconductors. Calculations done for various aspects e.g. influence of defects in a Mn doped GaAs system will be shown. Also, to explore the magnetism in a semiconducting host, we will show a comparative study of III-V, II-VI and IV-IV DMSs. Some comments about the exchange interactions in these systems will be made. Lastly, we will present a simple model to understand the magnetism in DMSs.

Electronic structure and Curie temperatures of diluted magnetic semiconductors

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Recent discovery of the carrier induced ferromagnetism in (In, Mn)As and (Ga, Mn)As encourages many experimental and theoretical studies on diluted magnetic semiconductors (DMS), because DMS are candidates for new functional materials whose magnetic properties are controllable by changing the carrier density. In this paper, the electronic structure of several III-V and II-VI DMS is calculated based on density functional theory, and an estimation of their Curie temperature ($T_c$) is given. The electronic structure is calculated by using the Korringa-Kohn-Rostoker method combined with the coherent potential approximation in order to describe
the substitutional and spin disorder. From the total energy differences between the ferromagnetic state and the spin-glass state, realistic estimations of Curie temperatures are achieved by using a mapping on the Heisenberg model in the mean field approximation. Carrier doping effects are also simulated by this method.

In (Ga, Cr)N, (Ga, Cr)As and (Ga, Mn)N, very large \( T_c \)'s above room temperature are predicted in realistic concentration ranges. In particular, it is found that the Cr-doped compounds are promising candidates for high-\( T_c \) ferromagnets. Room-temperature ferromagnetism is also predicted in (Zn, V)Se, (Zn, Cr)Se, (Zn, V)Te and (Zn, Cr)Te. It is also found that \( T_c \)'s decrease sharply by electron doping in (Ga, Mn)As and (Ga, Mn)N. In order to discuss the origin of the ferromagnetism, the Curie temperatures of Mn-doped GaN, GaP, GaAs and GaSb are systematically evaluated. Interestingly, they show very different concentration dependences. For low concentrations, the \( T_c \)'s are approximately proportional to the square root of Mn concentrations in GaN, GaP and GaAs. In particular, in case of GaN, a strong correlation between \( T_c \) and the half width of the impurity d-band is observed indicating that the double exchange mechanism dominates. On the other hand, \( T_c \) is almost linearly proportional to Mn concentration in (Ga, Mn)Sb. In this case, Mn-3d states have a negligible amplitude at the Fermi level, and the ferromagnetism is stabilized by the p-d exchange interaction. (Ga, Mn)P and (Ga, Mn)As are intermediate cases and it is difficult to say which mechanism dominates.
2nd Annual Meeting and Mid-Term Review

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POSTER SESSION
Ab initio study of electronic and magnetic structure of fcc Fe grown on a Cu(100) substrate.
B.Yu.Yavorsky, I.Mertig

Thin films of fcc Fe stabilized by epitaxial growth on a Cu(100) substrate have been a subject of great interest for both experimentlists and theoreticians. The question of the ground magnetic state of the fcc Fe, however, is still open. In the recent experimental study of Qian et.al [1] a non-collinear magnetic order in this system is discussed.

We have studied the electronic structure of the thin films of fcc Fe on a Cu(100) substrate theoretically by means of the screened KKR method. The system was modeled by a finite slab of 8 atomic layers of Cu sandwiched by 6 atomic layers of Fe on the both sides. The densities of states and the total energies of the ferromagnetic, the antiferromagnetic, and the non-collinear magnetic structure are presented. The possible magnetic ground state of the system is discussed.


Atomic contacts: stability, stress, electronic structure and magnetism
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Using KKR Green’s function method for low-dimensional systems and density functional theory we construct many body interatomic potentials for atomic contacts. Potentials are formulated in the second-moment tight binding approximation. The parameters of potentials are optimized simultaneously by including in the fit the results of the first principle calculations of selected cluster-substrate properties, forces acting on adatoms and ab initio bulk properties. We concentrate on the 3d atomic contacts. Atomic scale simulations reveal the interplay between the stability of nanocontacts, stress and electronic structure. We also discuss magnetic nanocontacts and show that that magnetic bridges can exhibit many interesting properties.

Spin motion in electron transmission through ultrathin ferromagnetic films
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The spin-dependent scattering of electrons at interfaces and ultrathin films has a considerable effect on the transport properties of ‘spintronic’ devices. In this contribution, we report on ‘theoretical experiments’ which provide direct access to the spin motion of electrons transmitted through 1–6 ML Fe on Pd(001). Spin- and angle-resolved photoelectron spectroscopy from core levels serves as microscopic probe. The spin polarization $P_{\text{in}}$ of the incoming photoelectrons (which were excited from a Pd core level) can easily be adjusted by choosing the incidence direction and the polarization of the incident light. Elastic scattering in the Fe films shows up as precession of the spin-polarization vector $\vec{P}$, whereas inelastic effects result in a rotation of $\vec{P}$ towards the magnetization $\vec{M}$. Significant structures in the constant-initial-state photoemission spectra are related to the electronic structures of the Pd substrate and of the Fe film.

**Beyond LDA: GW and SIC implementation in KKR**

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W.,M. Temmerman and Z. Szotek  
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B. Györfy  
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Ab-initio studies of semiconductors and insulators as well as of systems with strongly localized electrons entail great difficulties involved by the treatment of excitation energies and by many-body effects. The most successful first-principles method, the density-functional theory within the local-density approximation (LDA), is designed for ground-state properties and, hence, cannot provide a proper description of the electronic structures of semiconductors and insulators.

If localized electrons are present in the system, the LDA can be essentially improved by the self-interaction correction (SIC). This way, the self-interactions of single-particle charges, which are present in the LDA, cancel out for the localized electrons. However, SIC in conjunction with LDA is still not sufficient for a proper description of excitation energies and band gaps. For an accurate first-principles treatment, one would solve Hedin’s set of equations for the full Green’s function. Because a complete implementation of this formalism is very difficult, one usually neglects the vertex correction (random-phase approximation), and the self-energy is calculated within the $GW$ approximation (GWA). The non-self-consistent GWA was successfully implemented within several first-principles methods, but most of the existing implementations are generally designed for systems with delocalized electrons.

Here, a general *ab-initio* approach for the study of electronic properties of solids is presented. Basing on the Korringa-Kohn-Rostoker (KKR) method, we implemented the SIC for strongly localized electrons and the non-self-consistent GWA for the
inclusion of many-body effects. Our approach is illustrated by electronic-structure calculations for semiconductors and transition-metal oxides.

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

Electronic structure and tunnel magnetoresistance of Fe/MgO/Fe
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Understanding of tunneling magnetoresistance (TMR) is necessary for the important development and fabrication of magnetic tunnel junctions (MTJ) used in non-volatile memories (Magnetic RAM). A prototypical system for such a tunnel junction is Fe/MgO/Fe. It has the advantage that the insulating material is ordered and therefore well characterised. Recent work from an experimental group at the Max-Planck institute in Halle [Phys. Rev. Lett. 87 076102 (2001)] established that an FeO interface layer is grown between Fe and MgO and that a substantial interface relaxation takes place.

We have started a systematic study on how the electronic structure is affected by (1) interfacial structural relaxation, (2) oxidation of the Fe interface layer, (3) correlation effects in the FeO interface layer, and (4) non-stoichiometry in the FeO
interface layer. In conjunction with this we also investigate how these effects influence the tunnelling conductance. Our specific findings so far are: (1) structural relaxation at the interface induces an anti-parallel Fe spin magnetic moment in the layer adjacent to the Fe interface layer, (2) a substantially enhanced Fe spin moment in the interface layer is due to oxidation induced correlation effects, and (3) the spectral functions at the Fermi level with and without oxidation of the Fe interface layer differ quite dramatically.

In-plane uniaxial anisotropy at the Fe/ZnSe(001) interface
L. Nordström

We present a detailed study of the in-plane magnetocrystalline anisotropy (MCA) and its connection to the electronic bonding at an interface between a cubic ferromagnet and a cubic semiconductor, Fe/ZnSe(001). In particular, a uniaxial MCA is found. This is maybe surprising since the calculations are for perfect interfaces, but the effect is traced down to the $sp^3$-bonding between the semiconductor and the first monolayer of Fe. A uniaxial in-plane MCA is consistent with what is observed in general for bcc Fe/semiconductor interfaces, which has been a puzzle since its first observation. We will discuss our results in connection with existing models. It is also shown how this uniaxial symmetry is cancelled in a multilayer structures, leading to four-fold anisotropy. The calculations were performed using a full-potential linearized augmented planewave method (FP-APW+lo), which is a computationally more efficient version of the traditionally linearized metod, FLAPW. The spin-orbit induced MCA was studied through the force theorem, as well as through fully relativistic self-consistent calculations. The magnetic anisotropy is presented for several different Fe/ZnSe(001) systems, with three or five monolayers of Fe grown on a five atoms thick representation of the semiconductor, and with Zn terminated as well as Se terminated semiconductor interfaces.

An embedded Green-function approach to ballistic electron transport through an interface
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We present an efficient method for calculating the conductance of ballistic electrons through magnetic interfaces from first-principles using the embedding approach of Inglesfield [1]. In our method the Landauer-Buttiker formula [2] for ballistic transport is expressed in terms of two quantities that are available in the embedded Green-function formalism without additional calculations. One is the
embedding potential of bulk crystals on both sides of the interface and the other is the Green function in the interface region. The embedding formulation was implemented within the framework of the full-potential linearized augmented plane wave (FLAPW) method using the FLEUR code [3]. The actual implementation is discussed in detail. We will present calculations for magnetic multilayer structures used in giant magnetoresistance (GMR) and tunneling magnetoresistance (TMR) devices. In order to check the accuracy, and to allow a comparison with previous calculations we have chosen as an example of a GMR system, the Cu/Co/Cu(100) sandwich structure which is a model system in magneto-electronics and intensively investigated before. As a second application we present the investigation of the spin-resolved electronic tunneling through a Fe/MgO/Fe TMR junction.

3 http://www.flapw.de

Ballistic Spin Injection from Fe into ZnSe and GaAs
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We have investigated the ballistic spin injection from Fe into the semiconductors ZnSe and GaAs by means of an \textit{ab initio} method. The results show a very high spin polarization up to 99\% for the [001] growth direction and nearly no spin polarization for the [111] and [110] direction. The origin of the high spin polarization for the [001] direction are the different symmetries of the majority and minority spin wave functions. So we call it a symmetry enforced high spin polarization. This effect is absent for the other investigated directions, i.e., the [111] and [110] direction.

The calculation of the ground state properties is based on the density functional theory within the local density approximation and uses the screened KKR-Green’s function method. The conductance is calculated by the Landauer-Büttiker formula in a Green’s function description. We have investigated three different injection processes: (\textit{i}) the injection of hot electrons directly into the conduction band of the semiconductor, (\textit{ii}) the injection of thermal electrons at the Fermi energy without and (\textit{iii}) including a Schottky barrier at the interface.

If a Schottky barrier is included at the interface, new effects from resonant interface states can come in. They can dominate the tunnel current and can even change the sign of the current polarization, e.g., in the Zn terminated Fe/ZnSe(001) interface. Also we have calculated the interface resistance of the Schottky barrier in the (001) orientation as an input value for the analytical models of spin injection through a tunneling barrier proposed independently by Rashba and Fert \textit{et al}. By this we can roughly estimate the required thickness of the Schottky barrier to be 70\AA for Fe/ZnSe and 100\AA for Fe/GaAs(001).
Ab initio investigations of Fe/W(110): Magnetic Structure of Domain-Walls

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Atomically thin Fe films on the W(110) surface form a two-dimensional ferromagnetic domain structure. From experiments with spin-polarized STM it is known that the magnetization direction in the domains and the width of the walls between two adjacent domains are different for mono- and double-layer Fe coverage. For a mono-layer the wall width is on the atomic scale, while for a double layer the walls are extended over several atomic rows (around 8nm).

The shape of the walls is determined by the competition of the forces caused by spin-stiffness, spin-orbit coupling and magnetic dipolar interactions. In this poster we describe the walls with a simple model and investigate the possibilities and limits of obtaining the required parameters by ab initio calculations. The calculations are performed with the FLAPW-method based on density functional theory.

[e.g. M. Pratzer et. al. Phys. Rev. Lett. 87, 127201 (2001)]

Surface core level shift used as a tool to identify PdMn systems on Pd(100)
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Surface and interface core level shifts (CLS) of Pd 3d_{5/2} is calculated ab initio for the 1 ML Mn/Pd(100) system, as well as for three possible structures of reconstructed surface that may appear after annealing of the above system. The results are then compared to a recent experimental study by A. Sandell et al. (PRB 65, 035410 (2001)). The calculations are carried out in the framework of the interfaces KKR-ASA (CPA) Green’s function method. The shifts are calculated according to the complete screening picture which includes both initial state (electron energy eigenvalue) and final state effects (relaxation of the core-hole) in the same scheme. The effect of different types of magnetic ordering, ferromagnetic or antiferromagnetic, on the CLS of the as deposited and reconstructed samples was considered. From a comparison of calculated CLS with experiment, we identify which structure is actually present in experimental samples. Our conclusions agree with the work of A. Sandell et al., and point towards the same structure after annealing. We conclude that theoretical calculations of CLS provide a reliable tool for the solution of nonequilibrium structures at surfaces and interfaces.
Multiple-scattering theoretical approach to scanning tunneling spectroscopy

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The qualitative and quantitative theoretical description of scanning tunneling spectroscopy (STS) is usually based on the popular Tersoff-Hamann model. By simply relating the tunneling current to the spectral density of the sample, however, relevant properties of the tunneling through the tip-sample system are neglected.

Viewing electronic tunneling as a scattering process, we present a formulation of STS in terms of multiple-scattering theory which takes into account the tip-sample interaction. Further, electronic properties of the constituent systems can be obtained by ab-initio calculations. Besides a presentation of the general formalism and its implementation in a spin-polarised relativistic layer-KKR scheme, we sketch results for prototypical systems, with a focus on features of the scattering-theoretical approach.

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

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The development of magnetoelectronics has increased the interest in materials which can enhance the performance of spin-dependent devices. Such materials are the so-called half-metals which present a gap in the minority band resulting in 100% spin-polarization at the Fermi level. A significant number of the intermetallic Heusler alloys have been predicted to be half-metals. In this contribution we will present a complete study of both the bulk and surface properties of such Heusler alloys including both the families of the so-called half-Heusler alloys like NiMnSb and of the full-Heusler alloys like Co₂MnGe. Based on the ab-initio results for these compounds we will discuss the origin of the gap which is fundamental for the understanding of their electronic and magnetic properties. We will show that for both families of compounds the total spin magnetic moment \( M_t \) scales with the number of valence electron \( Z_t \), such that \( M_t = Z_t - 18 \) for the half-Heusler and \( M_t = Z_t - 24 \) for the full-Heusler alloys, thus opening the way to engineer new half-ferromagnetic Heusler alloys with the desired magnetic properties. Although the surfaces loose in-general the half-ferromagnetic character and exhibit a small degree of spin-polarization, we will show that in the case of compounds containing Cr, the large enhancement of the Cr moments at the surface reduces the effect of the surface states and leads to a very high spin-polarization of the surfaces, e.g. 84%
for the CrAl-terminated Co$_2$CrAl(001) surface or even 100% for the Cr-terminated CrAs(001) surface, so that these compounds might be promising for spindependent devices.

Electronic and magnetic properties of ferromagnet/semiconductor interfaces

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The electronic and magnetic properties of ferromagnet-semiconductor heterostructure systems have been studied using the scalar-relativistic KKR-CPA and fully-relativistic TB-KKR band structure methods. Concerning the resulting magnetisation profiles of multilayer and trilayer (FM/SC/FM) systems the most important features are that no magnetically dead layers occurred and an appreciable induced magnetisation was found in the semiconductor subsystem. Interdiffusion doesn’t lead to magnetically dead layers in the FM-layer and is energetically unfavourable. Investigating the hyperfine interaction and the magnetic circular dichroism (MCXD) more detailed information on the electronic structure could be obtained. Calculations of the interlayer coupling energy show interesting behaviour dependent on the thickness of the SC layer. Similar to metallic multilayer systems it could be shown that the magneto-crystalline anisotropy correlates with the anisotropy of the orbital moment.

The work has been based so far on unrelaxed ferromagnet-semiconductor heterostructures. In the near future investigations on the influence of lattice relaxations and interface reconstructions will be one of the issues of the project.


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Spin-dependent transport between two ferromagnetic electrodes separated by either an insulator or a semiconductor has received a lot of interest in the last years due to its potential technological applications. Recently it could be shown that a
measurable spin-polarised injection can be obtained in a TMR Fe/GaAs diode even at room temperature.

Many theoretical studies devoted to TMR systems can be found in the literature, but they either neglect relativistic effects or treat the crystalline structure in an approximate way. To allow for a most general description, our present investigations on FM/SC/FM systems have been performed within the framework of Tight-Binding Spin-Polarised Relativistic Multiple Scattering Theory (TB-SPR-KKR). The electronic structure and magnetic properties of Fe/GaAs/Fe as a representative example will be presented.

The transport properties of this systems are investigated by means of the Landauer-Büttiker formalism. The tunneling conductance and the TMR are calculated on a relativistic level. Model calculations allow us to gradually manipulate the strength of the spin-orbit coupling SOC and to investigate in detail its quantitative and qualitative influence on the spin-dependent transport.

**Probing magnetic susceptibilities using the field-induced magnetic circular dichroism**

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The magnetic circular dichroism in X-ray absorption (MCXD) is now a standard tool to probe the spin and orbital moments in magnetic materials by exploiting the so-called sum rules. In these systems the magnetic dichroism may be ascribed to the spontaneous exchange splitting. On the other hand, it is known that the magneto-optical Faraday effect, for example, can be observed for magnetic materials as well as for non-magnetic materials if they are exposed to a magnetic field. Accordingly, magnetic circular dichroism in X-ray absorption should be observable also in non-magnetic materials exposed to a magnetic field. A theoretical description of such an experiment is presented that is based on a combination of a fully relativistic linear response formalism and a corresponding treatment of magnetic circular dichroism. It is demonstrated that application of the magnetic sum rules now gives access to the spin and orbital element projected susceptibility of the system under investigation. In particular one finds that it is only the VanVleck contribution to the orbital susceptibility that is probed. In contrast to spontaneously magnetized systems, however, there are orbital contributions derived from the dichroic signal that stem from the external field and also from the intrinsic spin-orbit coupling. Illustrating examples will be presented for various transition metal systems that will demonstrate the usefulness and applicability of the new approach.

**Disorder-induced magnetism in TiFe\textsubscript{x}Co\textsubscript{1-x}**

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The transition metal system TiFe$_x$Co$_{1-x}$ has a CsCl-structure with Ti on one sublattice and a random distribution of Fe and Co according to the concentration on the other sublattice. From previous experimental investigations it was concluded that if this quasiorordered structure is formed, TiFe$_x$Co$_{1-x}$ is in a paramagnetic state. Only if a small numbers of Fe or Co atoms (1-2%) are occupying Ti sites (so called anti-sites) the alloy system gets a weak itinerant ferromagnet for $0.2 \leq x \leq 0.8$. To investigate this interesting disorder-induced magnetisation in more detail, we have used the Korkinga-Kohn-Rostocker (KKR) band structure method. The disorder in the system has been accounted for by means of the Coherent Potential Approximation (CPA). Our calculations demonstrated that TiFe$_x$Co$_{1-x}$ is indeed paramagnetic for all concentrations $x$ if these is no mixing of the two sublattices. Only a small mixing on the other hand gives rise to the formation of a spontaneous magnetisation that is in fairly good agreement with experiment. Our calculations give also a simple explanation for the puzzling Fe-Mößbauer data. While the Fe atoms on anti-sites have a large moment and hyperfine field, the hyperfine field of Fe-atoms on proper sites are very small because the valence band and core polarisation contributions nearly cancel another.

**LMTO Green Function approach for the *ab initio* calculation of the optical and magnetooptical properties of solids.**

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An approach for the calculations of the optical and magnetooptical properties of solids based on the one-particle Green Function introduced by Huhne and Ebert [1] and Szunyogh and Weinberger [2] is applied in the framework of the LMTO method. An advantage of the energy independent basis functions is explicitly taken into account which gives rise to the incredible acceleration of the calculations in comparison with the standard KKR scheme. At the same time the approach keeps all advantages of the more accurate KKR scheme as the possibility to account both for many-body effects and disorder effects in terms of the nonlocal energy dependent self energy. Preliminary results based on the simplified method of the Brillouin zone integration shows reasonably good coincidence with the standard methods for optical calculations based on the wave function formalism for Fe and Ni.


**Electron-electron interaction viewed by one-photon two-electron excitations**

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Theoretical and experimental evidence is provided that the spectrum of a photoexcited electron pair carries detailed information on the electron-electron interaction in metals. The theory is based on a two-particle LKKR approach that will be presented at the meeting. The main features found in the two-particle spectra have been assigned to (a) the exchange-correlation interaction, (b) the electronic band structure, (c) the photoelectron diffraction, and (d) the specific experimental setup. Comparison with experiments is made and common features and differences to the atomic case are pointed out.

Magnetization of the unsegregated and segregated (100) surface of MoV binary alloy

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Using ab initio total energy calculations in conjunction with statistical Monte Carlo simulations we have investigated magnetic properties of the (100) surface of the Mo_{25}V_{75}, Mo_{50}V_{50} and Mo_{75}V_{25} binary alloys both for homogeneous concentration profile and in the presence of surface segregations. While the MoV alloy is not magnetic in bulk in the whole range of concentrations, we predict a noticeable magnetization to occur at the top layer of the (100) surface. The surface segregations essentially enhance surface magnetization for Mo-rich alloys, so the average atomic magnetic moment is three times larger at the segregated surface in comparison with the homogeneous one. In order to find out an origin of the surface magnetization we have analyzed the alloy electronic structure.

First-principle study of the magnetoresistance effects in magnetic nanocontacts

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We present ab-initio calculations of the transport properties of the metallic atomic-sized nanocontacts. The nanocontacts were modeled by atomic chains of Co, Fe, Cu, Si, Al separating two semi-infinite magnetic Co-leads. We used the first-principle screened Korringa-Kohn-Rostoker method to calculate the electronic properties of the systems, treating the Co leads and atomic chains on the same
footing without any model parameters. The Landauer formalism was applied to investigate the conductance and magnetoresistance (MR). We found MR ratios of about 20-30

PHASE SEPARATION AT INTERFACES IN
La$_{2/3}$Ca$_{1/3}$MnO$_3$

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Mixed-valence manganites are oxides with perovskite structure and general formula AxA’1-xMnO3. They show a large number of properties originating from the many competing interactions between spin, charge and lattice. Therefore, they are very sensitive to structural modifications and to changes in the doping value, which can induce transitions from a magnetoelectronic phase to another. Among manganites, several compounds are half metallic ferromagnets whose high spin polarization is interesting for spintronics devices. For instance, very large magnetoresistance (MR) ratios are obtained in tunnel junctions at low temperature. However, the temperature dependence of the MR which decays much faster than magnetization and has prevented the observation of MR signal at room temperature so far. The precise cause of this behavior is unknown even if several studies suggest that it could be due to a loss of polarization at interfaces. Here, we report on magnetotransport and 55Mn NMR measurements of thin films of La$_{2/3}$Ca$_{1/3}$MnO$_3$ (LCMO) grown on SrTiO3 (STO) and on NdGaO3 (NGO) substrates, and on ceramic powders of La$_{2/3}$Ca$_{1/3}$MnO$_3$ with different grain sizes. Two lines are detected in the NMR spectra, indicating the presence of two types of regions with different conductivities. The detailed analysis of the data indicate that low-conductivity regions are more prominently located close to surfaces and interfaces. These data bring new elements for the understanding of the temperature decay of the MR of tunnel junctions and for the design of better manganite/insulator interfaces. Besides, the observation of parasite electronic phases close to surfaces or interfaces in La$_{2/3}$Ca$_{1/3}$MnO$_3$, a homogeneous compound in its bulk form, confirms the theoretical prediction of disorder-promoted phase separation.

Magnetic nanostructures on metal surfaces
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Magnetism, structure and interactions on the atomic scale are discussed. We present ab initio results on interatomic interactions between magnetic adatoms on a metal surface. We concentrate on Co adatoms and clusters on Cu(111) and Cu(100) surfaces. The scattering of surface state electrons by the Co adatoms on Cu(111) surface is studied by means of ab initio multiple-scattering KKR Green’s function method. The quantum interference between incident and scattered surface state electrons leads to standing waves in the electronic density around adatoms. Calculations resolve the lateral oscillations of the local density of states with a wavelength expected from the surface state band structure. Substrate-mediated long-range oscillatory interaction between adatoms is determined. Experimentally the direct observation of long-range interaction between adatoms up to 60 Angstrom distance is performed using pair correlations of diffusing adatoms recorded with a low temperature STM. The measured long-range interaction energies are in very good agreement with ab initio calculations.

Atomic relaxations in magnetic clusters are performed using ab initio based many body potentials constructed for a low-dimensional systems. Our results lead to the conclusion that the size-dependent mesoscopic mismatch, rather than the macroscopic one, is the driving force for strain-relieving effects at the mesoscale. The strain relief is predicted to have a profound effect on the shape of islands. Strain relaxation in Co islands leads to a reduced stress contribution in the partially filled layers. The stress in Co monolayers has been measured during epitaxial growth on Cu(001). The Co-induced stress is found to oscillate with a period of one atomic layer. Our experiments and atomic scale calculations ascribe the stress variation to the relaxation of epitaxial mesoscopic misfit strain in the islands.

The influence of hydrogen adsorption on magnetic properties of Ni/Cu(100) surface

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Ni/Cu(001) is known as a unique system showing the spin-reorientation transition (SRT) from an in-plane to out-of-plane magnetization direction when the Ni-overlayer thickness is increased. Recent experiments demonstrate that the critical thickness of the magnetization direction switching is strongly reduced by the H$_2$ adsorption. Here, the relaxed multilayer-structures have been investigated by the self-consistent all-electron full-potential linearized augmented plane-wave method
(FP-LAPW). The relaxed geometries, determined by total energy and atomic force calculations, show that H-monolayer (ML) strongly influences the interlayer distance between the Ni-surface and sub-surface layers yielding the outward relaxation of Ni-layer at H/Ni interface. Furthermore, a large decrease of local magnetic moments in the top surface area has been found if the surface was covered by H. Moreover, we present an ab-initio investigation of SRT. As a structural model we use the free-standing Ni-films and symmetric Ni/Cu/Ni-films covered by ML of H-atoms. Second, we calculate the magneto-crystalline anisotropy energy (MAE) employing the “magnetic force” theorem for the magnetization rotation. For fully relaxed Ni-films the SRT critical thickness of 4 ML is found in good quantitative agreement with the experiment. It is mainly caused by the reduction of Ni-film surface MAE due to the H-adlayer. Finally, we analyse the element specific contributions to the MAE using its relation with the anisotropy of the orbital magnetic moment.

Giant Magnetoresistance in carbon nanotubes

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(CN’s) are seamless graphitic cylinders \(^1\) with electronic properties which are sensitively related to their geometry. Spin-polarized transport in nanotubes is of a great interest since CN’s could play a role in future nanometer-scale electronic devices. We have studied Giant Magnetoresistance (GMR) in carbon nanotubes using the Landauer-Büttiker formula to calculate the differential quantum conductance and the GMR ratio for metallic and semiconducting carbon nanotubes. We consider two ferromagnetic regions with magnetization perpendicular to the tube axis, in contact with a non-magnetic finite-length nanotube. We calculate the change in conductance and hence the GMR ratio arising when the orientation of the magnetic moments changes from parallel to antiparallel. The Hamiltonian of our system is a parameterised four-state \((s, p_x, p_y, p_z)\) Hamiltonian based on a global fit to density functional results for graphite, diamond and \(C_2\) \(^2\). In order to calculate the conductance we use a general Greens function scattering technique\(^3\). The effects of a structural twist and a double barrier on GMR are studied and depending on the position of the Fermi energy, GMR ratios in excess of 200% are predicted.

Relativistic calculation of spin-wave spectra in thin magnetic films
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We have formulated a relativistic treatment to calculate the low energy magnetic excitation spectrum of thin magnetic films. The method can be considered as a relativistic generalization of the well known torque method by Lichtenstein et al. \cite{lichtenstein1987}, however, the mapping of the energy of the system onto a Heisenberg model is avoided. Our method can also supply well-defined layer resolved magnetic anisotropies. The method is demonstrated for ultrathin Fe films on Cu(100) and Au(100) surfaces as cases for an out-of-plane ground-state magnetization, while also for Co films on Cu(100) with an in-plane magnetization. The effect of the spin-orbit coupling can be seen, in particular, by inducing a gap in the long wavelength part of the magnon spectra and resulting in a clear difference in the spectrum along the (100) and (010) directions for the in-plane magnetized Co/Cu(100) system.

\cite{lichtenstein1987} A.I. Lichtenstein, M.I. Katsnelson, V.P. Antropov, and V.A. Gubanov, JMMM 67, 65-74 (1987)
Exchange interactions in magnetically frustrated systems

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Abstract

Recent ab initio calculations of volume dependences of magnetic properties for the most typical Invar system, a random fcc Fe-Ni Invar alloy, have shown that the evolution of the magnetic structure already at zero temperature is characterized principally by a continuous transition from the high-spin ferromagnetic state at high volumes to a disordered noncollinear configuration at low volumes [1]. This indicates the existence of large number of magnetic states in the system separated from each other by very small energy differences. Thus, the magnetic state in the system is highly frustrated. In this work we calculate from the first-principles [2] parameters of the classical Hiesenberg Hamiltonian for magnetic interactions in pure fcc Fe and fcc Fe-Ni alloys, the pair exchange parameters $J_{ij}$, as well as the effective exchange parameter $J_0$. We find that in pure Fe $J_0$ is almost completely dominated by $J_{ij}$ between nearest neighbors. We also show that there exists a particular area of volumes where more distant pair exchange parameters are big, of the order of $J_{ij}$ between the first nearest neighbors, but their contributions to the effective exchange parameter cancel each other almost exactly due to oscillating signs of these interactions. However, this peculiar behavior of exchange integrals disappears almost completely at Invar concentrations in Fe-Ni alloys. The origin of magnetic frustrations in random alloys is identified and discussed.

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