0.1 Report on the Conference "Computational Magnetism and Spintronics" - CompMag 2006

Forschungszentrum Jülich, Germany

October 2^{nd}-4^{th} 2006

Sponsors:
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Spintronics, magnetoelectronics and magnetism are currently among the most active research themes in condensed matter physics. These fields are progressing very fast and continue branching into increasingly wider areas of condensed matter. These include strongly-correlated electron systems as well as the connection to semiconductors in terms of diluted magnetic semiconductors, to organic molecules in terms of molecular magnets, to nanotubes, clusters and wires in the field of nano-spintronics and to ferroelectric materials in terms of multiferroics. The main objective of the Jlich conference was to bring together leading scientists in Europe, as well as guests from USA and Japan, being active in different fields of magnetism, in particular, in state-of-the-art first principles calculations. The conference provided grounds for active discussion on recent results as well as on future steps.

Program

Monday Oct. 2nd 2006

9:00-9:20	**Opening**	S. Blügel
9:20-11:00	**Session I: SPIN TRANSPORT AND MOLECULAR MAGNETISM (I)**	
9:20-10:00	*Spin transport through atoms and molecules from first principles*	S. Sanvito
10:00-10:20	*Density-functional study of Cr-based single molecule magnets*	V. Bellini
10:20-10:40	*Quantum transport through nanoscale contact*	T. Ono
10:40-11:00	*Computing STS by Layer-KKR real-space method*	K. Saha
11:00: 11:20	**Coffee break**	
11:20- 13:00	**SESSION II: DILUTED MAGNETIC SEMICONDUCTORS AND OXIDES (I)**	
11:20-12:00	*Diluted magnetic semiconductors: electronic and magnetic properties*	J. Kudrnovsky
12:00- 12:20	*Ab initio Design of Fabrication Process and Shape Control of Self-organized Tera-bit-density Nanomagnets in Dilute Magnetic Semiconductors by Two-dimensional Spinodal Decomposition*	T. Fukushima
12:20- 12:40	*Magnetic Transition Temperatures of Diluted Magnetic Semiconductors Calculated by the Cluster Approximation*	M. Ogura
12:40 - 13:00	*High Curie temperatures in (Ga,Mn)N from Mn clustering*	A. Ayuela
13:00 - 14:40	**Lunch**	
14:40 - 16:20	**SESSION III: MANY-BODY EFFECTS**	
14:40 - 15:20	*Ruthenates and other unconventional oxide magnets*	D. Singh
15:20 - 15:40	*Orbital physics in $LaVO_3$ and YVO_3*	E. Pavarini
15:40 - 16:00	*Variational Cluster Approach to the Electron Correlations in Half-Metallic CrO_2*	H. Allmaier
16:00 - 16:20	*Ab-initio approach to the lifetimes and inelastic mean free path of excited electrons in Fe, Ni, Pt and Au*	V. Zhukhov
16:20 - 16:50	Coffee break	

16:50 - 17:50	**SESSION IV: HALF-METALS**	
16:50 h - 17:10	*Thermal Collapse of Spin Polarization in Half-metallic Ferromagnets*	M. Lezaic
17:10 - 17:30	*Electronic structure and magnetism of spintronic materials*	B. Sanyal
17:30 - 17:50	*Role of stoichiometric and non-stoichiometric defects on the magnetic properties of half-metallic ferromagnet NiMnSb*	B. Alling
17:50 - 20:00	Poster session	

Tuesday Oct. 3rd 2006

9:00 - 10:40	**SESSION V: SPIN-TRANSPORT (II)**	
9:00 - 09:40	*Including Effects of Band Structure and Disorder in Spin Transport Calculations*	P. Kelly
9:40 - 10:00	*Spin-mixing conductances of thin magnetic layers*	I. Turek
10:00 - 10:20	*High TMR ratio in Fe/MgO/Fe junctions with even one atomic Fe layer*	P. Zahn
10:20 - 10:40	*Domain wall magnetoresistance in multilayers with large magneto crystalline anisotropy*	H. Herper
10:40 - 11:10	**Coffee**	
11:10 - 12:50	**SESSION VI: LOW-DIMENSIONAL MAGNETISM**	
11:10 - 11:50	*Nanomagnetism: theory and experiment*	O. Eriksson
11:50 - 12:10	*Orbital polarization in low dimensional transition metal systems*	C. Barreteau
12:10 - 12:30	*Magnetism of iron: from the bulk to the monatomic wire*	G. Autes
12:30 - 12:50	*Ab initio calculations of Co multi-wires on Pt(664)*	G. Bihlmayer
12:50 - 14:30	**Lunch**	

14:30 - 16:10	**SESSION VII: DILUTED MAGNETIC SEMICONDUCTORS AND OXIDES (II)**	
14:30 - 15:10	*Optimization of Tc in III-V DMS alloys using the LDA and GW approximations*	M. van Schilfgaarde
15:10 - 15:30	*Transport Properties of Half-Metallic Antiferromagnetic Diluted Magnetic Semiconductors*	H. Akai
15:30 - 15:50	*Spinodal Decomposition and Super-Paramagnetism in Dilute Magnetic Nitride Semiconductors*	K. Sato
15:50 - 16:10	*Nano-scale spinodal decomposition phase in ZnO-based dilute magnetic semiconductors*	M. Toyoda
16:10 - 16:30	**Coffee**	
16:30 - 18:10	**SESSION VIII: MULTIFERROICS AND COMPLEX MAGNETIC OXYDES**	
16:30 - 17:10	*Multiferroic Perovskite Oxides: A First-principles Study*	T. Oguchi
17:10 - 17:30	*First-principles calculation of optical properties of magnetic systems: Antiferromagnetic insulator MnO*	F. Bechstedt
17:30 - 17:50	*Unusual magnetic ground state in MnO under pressure*	K. Koepernik
17:50 - 18:10	*Materials design of $CuAlO_2$ based dilute magnetic semiconductors for semiconductor spintronics*	H. Kizaki

Wednesday Oct. 4th 2006

9:00 - 10:40	*SESSION IX: SPIN DYNAMICS AND RELATIVISTIC EFFECTS*	
9:00 - 9:40	*Relativistic treatment of spin currents and spin-transfer torques*	B. Gyorffy
9:40 - 10:00	*Noncollinear magnetism within OEP view to spindynamics*	S. Sharma
10:00 - 10:20	*Spiral magnetic structures driven by spin-orbit coupling: Determining the Dzyaloshinsky vector from first principles*	M. Heide
10:20 - 10:40	*Ab-initio ballistic conductance with spin-orbit coupling*	A. Dal Corso
10:40 - 11:10	**Coffee break**	

11:10 - 12:50	**SESSION X: EXCHANGE INTERACTIONS AND MAGNETISM IN COMPLEX MAGNETIC MATERIALS**	
11:10 - 11:50	*Competing interactions in the low-dimensional quantum magnet TiOCl*	R. Valenti
11:50 - 12:10	*Calculation of magnetic interactions in Cr spinel*	A. Yaresko
12:10 - 12:30	*The nature of the unusual sequence of phase transitions in MnAs: The first-principles study*	L. Sandratskii
12:30 - 12:50	*Complex magnetic order and transition to half-metallicity in Mn-doped Fe_3Si*	P. Mavropoulos

12:50 - 14:30 **Lunch**

Poster session

- **Poster with topic "Spin Transport"**
  - PI.1 A.K. Solanki *Quantum Conductance of Co-nanowires*
  - PI.2 D. Wortmann *All electron calculations of electronic transport: applications to magnetic tunnel junctions*
  - PI.3 V. Karpan *Efficient spin injection from a ferromagnet into a semiconductor*
  - PI.4 A. Calzolari *Ab initio electronic transport in spin-polarized systems*
- **II. Poster with topic "Diluted Magnetic Semiconductors and Oxides"**
  - PII.1 H. Katayama-Yoshida *Theory, new materials design and nano-process design of ferromagnetic semiconductors*
  - PII.2 A. Kashyap *Exchange Interactions in Dilute Magnetic Nitrides XN:Mn(X=Al, Ga, In)*
  - PII.3 D. Iusan *Theoretical study of the magnetic interactions in Mn-ZnO*
  - PII.4 V. A. Dinh *Pseudo-SIC and Monte Carlo study of the ferromagnetism in C (N)-doped Alkaline Earth Metal Oxides*
  - PII.5 L. Bergqvist *The search for new spintronic materials: half metallic antiferromagnetic diluted magnetic semiconductors*
  - PII.6 B. Belhadji *Exchange Interactions in Wide-Gap Dilute Magnetic Semiconductors*
  - PII.7 A.L. da Rosa *Electronic and magnetic properties of Cu-doped ZnO*
- **III. Poster with topic "Correlations, excitations, many-body effects, theory"**
  - PIII.1 P. Buczek *Non-adiabatic spin dynamics in thin magnetic films*
  - PIII.2 E. Gorelov *Numerically exact scheme for the electronic structure and magnetic properties of correlated systems*
  - PIII.3 S. Shallcross *Asymptotics of Exchange Integrals*
  - PIII.4 C. Friedrich *All-Electron GW Approximation in the Augmented-Plane-Wave Basis-Set Limit*
- **IV. Poster with topic "Half-metals"**
  - PIV.1 M. Ekholm *Effect of Mn surplus on the energetics and half-metallicity of NiMnSb*

- PIV.2 A. Beznogov *Calculation of interface properties for Heusler compounds*
- PIV.3 N. Baadji *Calculated Natural and Magnetic X-ray Circular Dichroism of Half-metal CrO_2*
- PIV.4 E. Sasioglu *Magnetic phase diagram of the Mn-based Heusler alloys from first-principles*
- PIV.5 A. Schindlmayr *Ab initio study of the electronic structure of magnetite*

- **V. Poster with topic "Low dimensional magnetism: wires, dots, surfaces, molecules, etc."**
  - PV.1 A. Horvath *Non equilibtrium transport through quantum dots*
  - PV.2 T. Wehling *Ab Initio Studies of Chromium Adatoms on W(110)*
  - PV.3 A. Ehesan *Dihydropyrene and polyacene couplers in Intramolecular magnetic interaction*
  - PV.4 S. Lounis *Non-collinear KKR Green function method: Application to 3d nanostructures on surfaces*
  - PV.5 Y. Mokrousov *Giant Magnetocrystalline Anisotropies of 4d Transition-Metal Monoatomic Chains*
  - PV.5 Dr. Nicolae Atodiresei *Tuning the magnetism of metal-benzene sandwiches*

- **VI. Poster with topic "Relativistic effects and other"**
  - PVI.1 S. Abdelouahed *Calculated x-ray magnetic dichroism of Gd at the L_{23} and M_{45} edges*
  - PVI.2 F. Tasnadi *Calculations for isolated slabs: MgO/Ag(001), Callen effective charge of O in MgO layers, polarization of $KNbO_3$ layers*

Abstracts

Spin transport through atoms and molecules from first principles

Stefano Sanvito
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The ingredients for a quantitative theory of quantum transport at the nanoscale are a non-equilibrium transport algorithm capable of evaluating the effects of a steady state current, and an electronic structure scheme. In addition if one requires the method to be scalable, the problem should be cast in a single-particle form. A possible solution is that implemented in our code Smeagol (www.smeagol.tcd.ie), which combines the Kohn-Sham Hamiltonian with the non-equilibrium Green's function (NEGF) method for transport. In this talk I will present several examples of the use of Smeagol in spin-transport problems,paying particular attention to the choice of exchange and correlation potential used (LDA, GGA, LDA+U or LDA+SIC). First I will review our recent progress on Fe/MgO/Fe tunneling junctions. I will discuss the bias dependence of the TMR, the effects of vacancies in the tunneling barrier, and I will provide a theoretical limit of the MgO thickness needed for useful technological applications. Then I will discuss our search for extremely large ballistic GMR in Ni atomic point contacts. In particular I will consider the effects of oxidation either in close proximity to the point contact or in the current-voltage probes. In contrast to several recent experiments, our theoretical analysis does not show any evidence of extremely large GMR of purely electronic origin. Finally I will demonstrate that magnetic spin-valves made from organic molecules sandwiched between Ni contacts have the potential for very large GMR. The conduction mechanism can vary from metallic to tunneling-like depending on the molecule chosen, and the GMR signal can be engineered by a clever choice of end groups.

Density-functional study of Cr-based single molecule magnets

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We present a density-functional study (DFT) of the magnetic interactions in Cr-based magnetic rings. This class of molecular nanomagnets, composed of heterometallic nanostructures with a cyclic shape and an antiferromagnetic exchange coupling between nearest neighbouring magnetic ions, have attracted much interest as they represent, when opportunely engineered, next-generation candidates for implementing qubit and quantum logic devices [1]. The systems we have focussed on, are ideal Cr8 rings as well as substituted, with Ni(II) ions, eterometallic rings. By mapping our ab-initio calculations, performed with the Wien2K code [2], onto classical effective Heisenberg spin Hamiltonians, the exchange interaction parameters have been extracted. We observe how in pure Cr8 rings, the inclusion of correlation effects in the Cr d orbitals by the GGA+U scheme (with U = 2.7 eV), reduces, as expected, the value of J, from J_{GGA} = 5.5 meV to J_{GGA+U} = 2.1 meV [3], improving the agreement with experiments, i.e. J_{Exp} = 1.5 meV [4]. We have also performed systematic calculations on Cr chain models, which modellize the magnetic interactions in Cr rings, by varying

the type of inorganic bridges between the paramagnetic centers, as well as the substituting divalent atom [5], and discuss the results comparing with the existent experimental literature. Our results support the idea that the magnetic interactions in ring-shaped Cr molecular magnets are well approximated by infinite chains analogue; such model systems can be more easily tackled in periodic DFT calculations than the real molecules and allow for a more systematic study of their electronic and magnetic properties.

[1] F. Troiani et al., Phys. Rev. Lett. 94, 207208 (2005); F. Meier, J. Levy and D. Loss, Phys. Rev. Lett. 90, 047901 (2003).

[2] P. Blaha et al., WIEN2K, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universitaet Wien, Austria), 1999. ISBN 3-9501031-1-2.

[3] V. Bellini, A. Olivieri and F. Manghi, Phys. Rev. B 73, 184431 (2006).

[4] J. van Slageren et al., Chem.-Eur. J. 8, 277 (2002).

[5] V. Bellini, et al., in preparation (2006).

Quantum transport through nanoscale contact

Tomoya Ono and Kikuji Hirose

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We demonstrate the results to elucidate a quantum transport properties of C_{60} molecules suspended between semi-infinite gold electrodes by first-principles calculations based on real-space method [1-3]. Our results indicate that the conductance of the C_{60} dimer is about 0.1 G_0 owing to the scattering of incident electrons at the junction between the molecules, whereas that of the C_{60} monomer is about 1 G_0. By encapsulating lithium atoms in their cages, the dimer exhibits good conductivity. The energy of the unoccupied molecular orbitals at the junction shifts down to the Fermi level, and as a consequence, the conductance of the Li@C60 dimer significantly increases. To explore the doping mechanism of the C_{60} bridges, we also compared the energy band structures of the infinite C_{60}, Li@C_{60}, and lithium chains and found that the Li@C_{60} chain is a conductor due to the electron transfer from the lithium atom to the fullerene, while the other chains are insulators. Our results indicate that the endohedral metal fullerene bridges have potential applications in spintronics devices when magnetic metals are encapsulated.

[1] K. Hirose, T. Ono, Y. Fujimoto, and S. Tsukamoto, First-Principles Calculations in Real-Space Formalism, Electronic Configurations and Transport Properties of Nanostructures, (Imperial College Press, London, 2005).

[2] T. Ono and K. Hirose, cond-mat-0606541.

Computing STS by the layer-KKR real space method

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A new method to compute scanning tunneling spectroscopy (STS) from first principles is proposed. The Green function of a tunnel junction is computed self-consistently within real-space multiple-scattering theory (layer-KKR), thus avoiding for example the artificial periodicity in a supercell approach. The conductance is then computed within the Landauer-Bttiker formalism. By this means, the electronic structure of realistic STM tips can be taken into account, hence going beyond the Tersoff-Hamann model. After introducing key issues of the new approach, its application to the Au(111) and c(2 x 2)-AFM Fe on W(001) surface will be discussed.

Electronic, Magnetic and Transport properties of diluted magnetic semiconductors

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We will review a parameter-free approach to determine electronic structure, exchange interactions, and thermodynamic and transport properties of diluted magnetic semiconductors (DMS). Magnetic and thermodynamic properties will be determined using two-step approach. In the first step, the selfconsistent electronic structure of a system is calculated from first principles while the effect of randomness is described in the framework of the coherent potential approximation (CPA). The calculated total energies connected with small rotations of spins are then mapped onto the classical Heisenberg Hamiltonian using the magnetic force theorem. The exchange interactions between magnetic atoms are obtained and their properties will be discussed in detail. In the second step, statistical properties of the Heisenberg Hamiltonian are studied with a special attention devoted to the determination of critical temperatures using a newly developed selfconsitent local random-phase approximation. The magnetic properties of DMS are dominated by short ranged interatomic exchange interactions that have a strong directional dependence suggesting that the ordering of DMS is strongly influenced by magnetic percolation effects. The observed critical temperatures of a broad range of DMS are reproduced with a good accuracy only when the magnetic atoms are distributed randomly on the lattice. Calculated electronic structure is also used to determine the transport properties of (Ga,Mn)As diluted magnetic semiconductors using a linear response theory in which the disorder-induced vertex corrections are determined within the CPA. Results for both the bulk and layered (Ga,Mn)As semiconductors will be compared and the relevance of vertex-corrections will be discussed.

Ab initio Design of Fabrication Process and Shape Control of Self-organized Tera-bit-density Nano-magnets

in Dilute Magnetic Semiconductors by Two-dimensional Spinodal Decomposition

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Due to the discovery of carrier induced ferromagnetism in dilute magnetic semiconductor (DMS), people try to realize semiconductor spintronics devices by using the ferromagnetic DMS. The requirement for the realization of the semiconductor spintronics is to develop the fabrication method of Tera-bit-density nano-magnets using the self-organization by bottom-up nanotechnology, the control method of growth position in the atomic scale for the system integration on the semiconductor substrate, and the shape-control method of the Tera-bit-density nano-magnets for the application of spintronics devices in the DMS. In this work, a new fabrication process in a bottom-up nanotechnology to realize self-organized Tera-bit-density nano-magnets is designed based on ab initio calculations of effective pair interactions between magnetic impurities in the DMS and on Monte Carlo simulation of layer-by-layer crystal growth. We show that growth positions, shape and density of quasi-one-dimensional nano-magnets in the DMS can be controlled by the nano-scale seeding on the semiconductor substrate and the vapor pressure or concentration of the doped magnetic impurities under the thermal non-equilibrium crystal growth condition, such as molecular-beam epitaxy, metal-organic vapor phase epitaxy or metal-organic chemical vapor deposition.

Magnetic Transition Temperatures of Diluted Magnetic Semiconductors Calculated by the Cluster Approximation

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Many theoretical investigations on magnetic diluted semiconductors (DMSs) have been done in this decade. In particular, the magnetic transition temperatures TC have been discussed intensively aiming at the practical application of DMSs. In such calculations, the approaches using the Monte Calro simulations together with the calculated exchange coupling constant J_{ij} becomes a standard instead of the mean field approximation, which sometimes overestimates TC. Although the Monte Calro simulations can give reasonable results, it is rather time consuming. In the present study, we introduce the calculation of the transition temperature using the extended cluster approximation [1]. We calculated the electronic structure and TC of various DMSs using the KKR-CPA-LDA method. As for the transition temperature, the cluster approximation gives very accurate results with far less computational effort than MC simulations. We discuss the

efficiency of the method and the transition temperatures TN of the half-metallic antiferromagnetic semiconductors [2] calculated by this method.

[1] H. Mano, Prog. Theor. Phys. 57 (1977) 1848.
[2] H. Akai and M. Ogura, PRL 97 (2006) 026401.

High Curie temperatures in (Ga,Mn)N from Mn clustering

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The effect of microscopic Mn cluster distribution on the Curie temperature (T_C) is studied using the spin-polarized total energy density functional calculations with the projector augmented wave method. We find that the calculated T_C depends crucially on the microscopic cluster distribution [1]. The partially dimerized Mn2-Mn1 distribution is found to give the highest TC. In general, the presence of the Mn2 dimer has a tendency to enhance T_C. The lowest T_C values are obtained for the Mn4 -Mn1 and Mn4-Mn3 distributions. In general, the presence of the symmetric Mn4 tetramer has a tendency to suppress T_C to very low temperatures.

[1] Teemu Hynninen, Hannes Raebiger, J. von Boehm, and Andres Ayuela Appl. Phys. Lett. 88, 122501 (2006)

Ruthenates and Other Unconventional Oxide Magnets

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The study of correlated electron physics in transition metal oxides traditionally emphasizes 3d materials. 4d and 5d oxides get less attention, though recently rather fascinating physics has been found in them, e.g., triplet superconductivity in Sr_2RuO_4. They generally have weaker on-site Coulomb interactions relative to hopping; this leads to a greater role for band structure effects, as seen, e.g., in the robust k-dependent spin fluctuations in Sr_2RuO_4, and the sensitivity of the electronic state to lattice structure [4]. In fact, these features: greater interplay of band structure with correlation effects and greater coupling of spin and charge degrees of freedom are key to many differences between 3d and 4d and5d oxides. These differences lead to novel states, not seen in the more Hubbard-like 3d oxides, Sr_2RuO_4 being an example. Furthermore, relativistic effects are much more important in these materials, than in 3d magnets. Thus extremely large magneto-crystalline anisotropies and magneto-optical coefficients can be expected. Here the physics of ruthenates and related oxide magnets is discussed from the point of view of electronic structure calculations. A key point is the

importance of O in the magnetic and other properties due to strong metal O hybridization.

The work described here was in collaboration with I.I. Mazin and S.V. Halilov. This work was supported by the Department of Energy.

Orbital physics in $LaVO_3$ and YVO_3

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We calculate the electronic structure of LaVO3 and YVO3. By using the first-principles downfolding method, we construct a low energy Hubbard Hamiltonian for the t2g bands; we solve this Hamiltonian using the dynamical mean field theory. The calculated Hubbard bands and Mott gaps are in very good agreement with experimental spectroscopy data. We show that, while in YVO3 orbital fluctuation are already suppressed at room temperature, in LaVO3 they are suppressed only in the low temperature monoclinic phase. We argue that, at room temperature, LaVO3 is very close to an orbital liquid.

Variational Cluster Approach to the Electron Correlations in Half-Metallic CrO_2

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For future high-performance spintronic devices, it is highly desirable to explore and understand the ground state of half-metallic ferromagnetic (HMF) materials in the presence of electron-electron correlations. A useful theoretical tool to investigate electronic and magnetic properties of HMF is based on first-principle band-structure calculations. In order to capture local - but dynamic - many-body correlations, the Local Density Approximation (LDA) was combined with Dynamical Mean Field Theory (DMFT). Even though recently, LDA+DMFT achieved significant progress in the microscopic description of HMF, further development should include non-local solvers of the many-body problem Therefore, we propose a Variational Cluster Approach (VCA) in combination with realistic electronic structure as a method which allows to include non-local correlation effects. Several LDA+VCA results applied to CrO_2 are presented.

Ab-initio approach to the lifetimes and inelastic mean free path of excited electrons in Fe, Ni, Pt and Au

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The transport of excited electrons in ferromagnetic and noble metals in an essential aspect of the physics of magneto-electronic devices. A characteristic

crucial for creating new devices (spin-valve transistors, magnetic tunnel transistors) is the attenuation length of excited electrons at low excitation energy which is governed by the processes of inelastic and elastic electron-electron scattering. We develop a first-principle method for the calculation of inelastic mean free path (IMFP) of excited electrons in metals and apply it to Fe, Ni, Pt and Au. IMFP is defined as product of group velocity and inelastic lifetime of excited electrons. The group velocity is evaluated from band-structure calculations. The lifetime of an excited electron is also calculated from first principles basing on the self-energy formalism of many-body theory. The lowest-order term of the theory (GW term) accounts for the decay of excitation through the interaction between the excited electron and polarization field. The high-order terms (T-matrix-terms) include multiple scattering between the excited electron and secondary electrons and holes [1]. For ferro-magnetics by means of T-matrix term the effect of magnon generation on the lifetime is accounted for [2]. We show that the effect of magnon generation in Fe and Ni is essential for lifetimes and IMFP at excitation energy below 1 eV. We calculate the energy dependence of the spin asymmetry of IMFP in Fe and interpret it basing on the densities of electronic states. For Pd and Au in accordance with experiment we find, respectively, rather low and very high values of IMFP and explain it from the features of the band structure. We show that the energy and spin dependence of lifetimes is in good correspondence with a simple random k which is based on a convolution of density of states.

[1] V.P. Zhukov, E.V. Chulkov, P.M. Echenique. Phys. Rev. B 72 (2005) 155109

[2] V.P. Zhukov, E.V. Chulkov, P.M. Echenique. Phys. Rev. Lett. 93 (2004) 096401

Thermal Collapse of Spin Polarization in Half-metallic Ferromagnets

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Half-metallic ferromagnets (HMF) are ferromagnetic metallic compounds showing, under ideal circumstances, e.g. at zero temperature and no structural disorder, a spin-polarization P of 100We follow two approaches to the excited magnetic states. The first approach is based on the full-potential linearized augmented plane-wave (FLAPW) method[1]. Using the force theorem we deduce magnon dispersion relations. A subsequent Fourier transformation yields the real-space exchange constants Jij of the Heisenberg model. We use a Monte Carlo method to find the thermodynamic quantities, such as the magnetization curve M(T), susceptibility and the Curie temperature TC. The second approach is based on the disordered local moment (DLM) state $NiMn_{1-x}Mn_xSb$, with 0 < x < 0.5 representing the temperature range 0 < T < TC. This approach describes the system at T¿0 in a mean-field manner. The DLM calculations are done within the coherent-potential approximation (CPA) and the Korringa-

Kohn-Rostoker full-potential Green function method[2]. For multicomponent HMF we cannot confirm the proposed model which assumes that P(T)? M(T)[3]. The presence of different magnetic components can, in principle, lead to a drop of the spin-polarization at T¿0 which is much faster than the drop of magnetization in these systems. This effect can be quite drastic and depends largely on the strength of the hybridization among the components[4] We describe the effects of temperature in more detail for the compounds NiMnSb and Co_2MnSi.

[1] The FLEUR code, http://www.flapw.de

[2] The SPR-TB-KKR package, H. Ebert and R. Zeller, http://olymp.cup.uni-muenchen.de/ak/ebert/SPR-TB-KKR

[3] R. Skomski and P. A. Dowben, Europhys. Lett. 58, 544 (2002)

[4] M. Lezai¸ Ph. Mavropoulos, J. Enkovaara, G. Bihlmayer, and S. Bluegel, Phys. Rev. Lett. 97 , 026404 (2006)

Electronic structure and magnetism of spintronic materials

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Half-metallic ferromagnets with high Curie temperatures are valuable ingredients for spintronics applications. In this respect, diluted magnetic semiconductors and other stoichiometric ferromagnetic compounds have received enormous attention in theoretical and experimental research for the last few years. As the physics of these systems is extremely complicated, a theoretical understanding in the microscopic scale is an absolute necessity. Here, we present ab-initio calculations on diluted magnetic semiconductors and other half-metallic ferromagnets. The two systems considered are zinc-blende MnAs and half-Heusler Mn doped NiTiSn. We will show results on the calculations of Curie temperatures using Monte-Carlo simulations with effective Heisenberg Hamiltonian within the framework of ab-initio methods. Volume effects on the exchange interaction parameters and hence Curie temperatures will be presented too.

Role of stoichiometric and non-stoichiometric defects on the magnetic properties of half-metallic ferromagnet NiMnSb

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The first material to be predicted from first-principles calculations as half-metallic was NiMnSb and the research on this material has been intense due to its possible applications in spintronics devices. The failure of many experiments to measure spin polarization to more than a fraction of the predicted 100 % has partly been blamed on structural defects. In this work a complete first-principle treatise of point defects, non-stoichiometric anti-site, interstitial

and vacancy defects, as well as stoichiometric atomic swap defects in NiMnSb is presented. We find that the formation energies of the defects span a large scale from 0.2 to 14.4 eV. The defects with low formation energies preserve the half-metallic character of the material. We also find that some of the defects increase the magnetic moment and thus can explain experimentally observed increase of magnetic moments in some samples of NiMnSb. Most interesting in this respect are Mn interstitials which increase the magnetic moment, have low formation energy and keep the half-metallic character of the material.

Including Effects of Band Structure and Disorder in Spin Transport Calculations

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I give a brief overview of the wave-function matching method for calculating scattering matrices from first-principles that has been implemented in Ywente using (i) a TB-MTO basis which in the Atomic Spheres Approximation is suitable for close-packed structures and (ii) a real-space grid method suitable for open structures such as atomic wires. The methods are illustrated for a variety of recent applications such as atomic wires, magnetic tunnel junctions, spin injection etc.

Spin-mixing conductances of thin metallic layers

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The spin-mixing conductance is a complex quantity that (along with the usual spin-resolved conductances) provides a complete information on a linear response of the currents and spin currents at a ferromagnet/non-magnet interface due to the bias and spin accumulation inside the two adjacent materials [1]. We consider a thin ferromagnetic layer attached epitaxially to two non-magnetic leads and formulate the spin torque and spin currents due to the spin accumulation in one of the lead. We use a non-equilibrium Green's function approach, show a relation to the scattering (Landauer-Buttiker) theory, and describe an implementation within the tight-binding linear muffin-tin orbital (TB-LMTO) method combined with the coherent-potential approximation (CPA) for substitutionally disordered systems [2]. The developed theory is applied to simple systems (Cu/Co/Cu) and to more complex systems based on: a random NiFe alloy (permalloy), the halfmetallic ferromagnet Co_2MnSi, and the diluted magnetic semiconductor (Ga,Mn)As. Particular attention is paid to the thickness dependence and to effects of disorder.

[1] A. Brataas, G.E.W. Bauer, P.J. Kelly: Physics Reports 427 (2006) 157.
[2] K. Carva, I. Turek, J. Kudrnovsky, O. Bengone: Physical Review B 73 (2006) 144421.

High TMR ratio in Fe/MgO/Fe junctions with even one atomic Fe layer

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Recent experiments [1] based on epitaxially grown Fe/MgO/Fe samples shed light on the microscopic origin of tunneling magnetoresistance (TMR). First of all, the obtained TMR ratios exceeded the predictions by Julliere's model. Second, the bias voltage characteristic shows features which could be related to the electronic structure of the system. The aim of this contribution is to demonstrate how the interface structure, the barrier thickness, and the finite thickness of the Fe electrode layers influence the TMR ratio and the corresponding bias voltage dependencies. Three junction geometries are considered with ideal interfaces and with a mixed Fe oxide layer experimentally found at the Fe/MgO interface. A screened Korringa-Kohn-Rostoker (KKR) method based on density-functional theory was applied to calculate the electronic and magnetic structure of the different junctions self-consistently. The Landauer conductance of planar junctions was calculated using the Baranger-Stone scheme by means of Green's functions. The bias dependence of the tunneling conductance and the magnetoresistance were computed in the limit of coherent transport. Positive and negative TMR ratios are obtained as a function of interface structure and even a sign reversal of TMR as a function of bias was found [2]. The results demonstrate that the current voltage characteristic is dominated by the interface electronic structure rather independent on the barrier thickness. Finally, junctions with finite Fe layer thicknes and non-magnetic leads will be discussed. It will be shown that the leads have just to provide states of ?1 symmetry which tunnel most efficiently across the barrier and the spin-filter effect is generated by even one monolayer of Fe [3].

[1] J. Faure-Vincent et al., Appl. Phys. Lett. 82, 4507 (2003), S. Yuasa et al., Nature Materials 3, 868 (2004), S.S.P. Parkin et al., ibid., 862 (2004).
[2] C. Heiliger et al., Phys. Rev. B 72, 180604(R) (2005), C. Heiliger et al., Phys. Rev. B 73, 214441 (2006).
[3] C. Heiliger et al., subm. to Phys. Rev. Lett. (2006).

Domain wall magnetoresistance in multilayers with large magneto crystalline anisotropy

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Domain walls in magnetic thin films occurring at the interfaces of grains with different magnetic orientation significantly influence the electronic properties of magnetic multilayers. In view of electrical devices operating with the help of magnetic films the question of the influence of domain walls on, e.g., the magnetoresistance (MR) has attracted much interest. Several experiments on FM thin films or systems with constricted domain walls showed that domain walls should give an additional contribution to the GMR [1,2]. Hassel et al. have investigated the domain wall magnetoresistance (DWMR) in CoPt films and found a DWMR of ?1%, which is of the same size as the anisotropic MR[3]. We investigated the MR and the energetic properties of fcc Co and $Co_{80}Pt_{20}$ films which are embedded between two semi-infinite Pt systems acting as constraints for the domain walls and electron reservoir. Additional calculations have been performed for systems with a finite Pt film on top, which corresponds to the experimental configuration. Co and $Co_{80}Pt_{20}$ possess a large magneto-crystalline anisotropy and, therefore, the width of the domain walls is expected to be relatively small. This makes them interesting for perpendicular recording, i.e., future storage devices[4]. A fully relativistic version of the screened Korringa-Kohn-Rostoker method has been used to investigate the electronic properties of the layered structures. In order to describe Bloch domain walls in the magnetic films we follow the technique of Schwitalla et al.[5]. The magnetoresistance is investigated by using a Kubo-Greenwood approach. Assuming perpendicular geometry, for which the magnetic moments are in-plane oriented and the current is adjusted parallel to the surface normal allows a direct calculation of the DWMR. The calculations of the DMWR have been performed depending of the width of the domain wall and the thickness of the FM layer. Our results are compared to the conclusions from model calculations[7]

[1] G. Dumpich, T. P. Krome, B. Hausmanns, J. Magn. Magn. Mater. 248 241 (2002).

[2] J. L. Prieto, M. G. Blamire, J. E. Evetts, Phys. Rev. Lett. 90 027201 (2003).

[3] C. Hassel, G. Dumpich, to be published.

[4] J. Ariake, T. Chiba, S. Watanabe, N. Honda, K. Ouchi, J. Magn. Magn. Mater. 287 229 (2005).

[5] J. Schwitalla, B. L. Gyorffy, L. Szunyogh, Phys. Rev. B 63 104423 (2001).

[6] L. Szunyogh, B.Ujfalussy, P. Weinberger, Phys. Rev. B 51 9552 (1995).

[7] P. M. Levy, S. Zhang, Phys. Rev. Lett. 79, 5110 (1997).

Nanomagnetism, theory and experiments

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The magnetic properties of selected nano-sized systems will be presented. Both magnetic clusters supported on a surface as well as precipitates of magnetic clusters in a non-magnetic host have been studied by first principles theory, and

when possible compared to experimental data. The possibility to form non-collinear magnetic arrangements will be discussed, especially for clusters with a possibility to form frustration.

Orbital polarization in low dimensional transition metal systems

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We have developed a TB Hamiltonian, including spin-orbit coupling, with electron-electron interactions described by a multiband intra-atomic Hubbard Hamiltonian treated in the Hartree-Fock approximation, for magnetic transition metals[1]. The basis set is limited to d orbitals. Contrary to most previous works, all terms arising from the Hartree Fock decoupling of the electron-electron interactions are taken into account. These terms introduce diagonal as well as non diagonal intrasite matrix elements in the Hamiltonian which are calculated with the full set of Coulomb interaction matrix elements, i.e. involving one, two, three, and four different orbitals. In this "full" model the orbital polarization (OP) effects are naturally taken into account. It is then compared to simplified Hamiltonians in which the OP effects are included by adding a term proposed by Eriksson et al[2] proportional to L2, treated in meanfield (orbital polarization ansatz: OPA). We have applied our models to low dimensional systems (Fe wires and clusters). A drastic increase of the orbital moment and magneto-crystalline anisotropy energy (MAE) is found compared to the bulk. It will also be shown that, with simplified Hamiltonians and in saturated systems, the OPA yields the right tendency of increasing the orbital moment and MAE in agreement with the full scheme, eventhough some discrepancies exist in the band structure. The validity of the OPA is however seriously questionnable in unsaturated systems for which both spin and orbital moments as well as MAE are badly reproduced. We are now planning to extend our model to more complex systems in a realistic s, p and d basis set.

[1] Is the orbital polarization ansatz justified? M.C. Desjonqueres, C. Barreteau, G. Autes, and D. Spanjaard. Submitted to Phys. Rev. Lett.

[2] Eriksson, M.S.S. Brooks and B. Johansson, Phys. Rev. B 41, 9087 (1990).

Magnetism of iron: from the bulk to the monatomic wire

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The magnetic properties of iron (spin and orbital magnetic moments, magnetocrystalline anisotropy energy) in various geometries and dimensionalities are investigated by using a parametrized tight-binding model in an s, p and d atomic orbital basis set including spin polarization in a simplified Stoner-like model and the effect of spin-orbit coupling[1]. The validity of this model is well

established by comparing the results with those obtained by using an ab-initio code. This model is applied to the study of iron in bulk bcc and fcc phases, (110) and (001) surfaces and to the monatomic wire, at several interatomic distances. New results are derived. The variation of the component of the orbital magnetic moment on the spin quantization axis is studied as a function of depth, revealing a significant enhancement in the first two layers, especially for the (001) surface. It is also found that the magnetic anisotropy energy is drastically increased in the wire and can reach several meV. This is also true for the orbital moment, which in addition is highly anisotropic. At equilibrium distance the easy magnetization axis is along the wire but switches to the perpendicular direction under compression. The agreement with ab-initio calculations is almost perfect and demonstrates the good transferability of the parameters and the adequacy of the model. This opens up the possibility of obtaining accurate results on other elements and systems with much more complex geometries (clusters, break junctions etc..) at least when the coordinence of the atoms is not too low. Indeed at very low coordinence both ab-initio calculations and our tight-binding model must be corrected for orbital polarization effects which are the subject of another abstract submitted to this conference (Orbital polarization in low dimensional transition metal systems).

[1] Magnetism of iron: from the bulk to the monatomic wire, G. Autes, C. Barreteau, D. Spanjaard and M.C. Desjonqueres, J. Phys: Condens. Matter 18 (2006), 1-29.

Ab initio calculations of Co multi-wires on Pt(664)

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We investigate Co wires of different width deposited on step-edges of Pt(111), simulated by a Pt(664) surface. The calculations were preformed in the framework of the density functional theory using the FLAPW method. The magnetic properties of an adsorbed Co chain showed a magnetic anisotropy energy (MAE) and easy axis in good agreement with experimental data [1]. Inclusion of relaxations turned the easy axis even more in the direction of the upper terrace and quenched the orbital moments and their anisotropy [2]. While this seems unfavorably in comparison to experiment, we argue – based on a decomposition of the contribution to the MAE of the different atoms (Pt or Co) – that relaxations might be an essential part of calculations including orbital polarizations. We investigated also the evolution of the easy axes and the MAE as function of the number of Co chains deposited on the stepped surface. The results nicely compare to those obtained experimentally [3]. We present a simple model to account for the experimentally observed oscillations of the easy axis [4].

[1] P. Gambardella et al., Nature 416, 301 (2002)

[2] S. Baud et al., Phys. Rev. B 73, 104427 (2006)

[3] P. Gambardella et al., Phys. Rev. Lett. 93, 077203 (2004)

[4] S. Baud et al., Surface Science (in press) (2006)

Optimizing Tc in III-V DMS alloys using the LDA and GW approximations

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Dilute Magnetic semiconductors are a new but little understood class of materials, and in particular the origin of ferromagnetism in these materials. As we will show, the LSDA combined with the rigid-spin approximation fails to predict the observed magnetism in many of these materials, and a key question is whether the failing is due to the approximations made, or is something else going on? The best understood of DMS is zincblende $Mn_xGa_{1-x}As$, with x ¡ 0.1. Optimally grown thin films have been recently shown to exhibit conventional M(T) behavior with Tc of about 170 K. This was modelled with quasirandom structures of large supercells, using a standard LDA linear-response technique. Temperature-dependence was using a form of the Cluster Variation method for the Heisenberg model. The calculated Tc is predicted to increase with x to x =15 To address whether the LSDA+rigid spin, or the assumption of ideal random alloys is in error, a recent implementation of self-consistent GW calculation of the spin susceptibility is presented for some Mn- and Cr- bearing semiconductors. The scGW approach is shown to to accurately describe the electronic structure of d systems, even NiO and f systems where the LDA fails. We show while the LSDA poorly predicts the magnetic moment of bulk NiO and MnAs (NiAs phase), scGW predicts them accurately, and signficantly alters the Fermi surface and magnetic moment. When applied to MnxGa1-xAs the Mn d levels shift in a similar manner, and agree with photoemission data. The effect of scGW on the magnetic exchange interactions in various DMS-like compounds of Mn and Cr is in progress and will be described.

Transport Properties of Half-Metallic Antiferromagnetic Diluted Magnetic Semiconductors

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Recently, it is pointed out that half-metallic antiferromagnetism might be possible for the diluted magnetic semiconductors. A striking feature of these systems is that they carry no magnetization and yet are half-metallic. This feature opens up a possibility of using these systems for the spintronics devices that can be operated, owing to the smallness of the magnetic anisotropy, by weak electric current. For such systems to be useful, however, it is crucial that the electric current reflects their magnetic structure sensitively. Such transport properties of such systems are also interesting because they represent a new

type of magnetic system: The half-metallic antiferomagnetism actually is a special case of disordered ferrimagnetism with compensated magnetization. The purpose of the present study is to discuss the transport properties of such half-metallic diluted antiferrmomagnetic semiconductors and their films on the basis of systematic calculation using the Green function method combined with the coherent potential approximation (CPA) and Kubo-Greenwood formula. A particular interest is in the effects of anti-phase boundary of the magnetic domains on DC conductivity. We examine such effects and discuss the possibility of using half-metallic antiferromagnetic diluted magnetic semiconductors for spintronics.

Spinodal Decomposition and Super-Paramagnetism in Dilute Magnetic Nitride Semiconductors

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Today, it becomes possible to reproduce experimental Curie temperatures (TC) of dilute magnetic semiconductors (DMS) such as (Ga, Mn)As and (Zn, Cr)Te accurately from first-principles [1]. In contrast to this success, agreement between the theory and experiments is not satisfactory in wide band gap DMS such as nitride DMS, and more realistic description of wide band gap DMS is needed. For example, in general, DMS systems have solubility gap and in thermal equilibrium they show phase separation (spinodal decomposition), however in the previous theoretical approaches homogeneous impurity distribution is assumed [1]. In this paper we focus on the spinodal decomposition in nitride DMS, and study how inhomogeneous impurity distribution affects the ferromagnetism. We calculate electronic structure of nitride DMS from first-principles by using the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. Then, chemical pair interactions between magnetic impurities in the effective CPA medium are estimated by using the generalized perturbation method proposed by Ducastelle et al. Magnetic exchange interactions are calculated by the Liechtensteins method [1]. The spinodal decomposition of DMS is simulated by the Monte Carlo method. Curie temperatures of simulated spinodal decomposition phases are calculated by the random phase approximation [2]. It is shown that above the percolation threshold the system is ferromagnetic and TC goes up during the decomposition process [3]. For low concentrations, the system is super-paramagnetic (TC =0) because small isolated clusters are formed in DMS due to the decomposition. However, the Monte Carlo simulation for the magnetization process of the decomposition phases indicates that super-paramagnetic blocking temperature could be higher because the activation energy to flip the magnetization becomes larger for the decomposition phases. Finally, we take into account a MBE crystal growth condition in our simulations and show that under this condition, quasi-one-dimensional structures of impurities are formed even for low concentrations [4]. This simulation could explain the ferromagnetic behavior of wide gap DMS at high temperature.

1. L. Bergqvist et al, Phys. Rev. Lett. 93, 137202 (2004), K. Sato et al., Phys. Rev. B 70, 201202 (2004), T. Fukushima et al., Jpn. J. Appl. Phys. 43, L1416 (2004)
2. S. Hilbert et al., Phys. Rev. B 70, 165203 (2004)
3. K. Sato et al., Jpn. J. Appl. Phys., 44, L948 (2005)
4. T. Fukushima et al., Jpn. J. Appl. Phys., 45, L416 (2006)

Nano-scale spinodal decomposition phase in ZnO-based dilute magnetic semiconductors

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As it is now, Curie temperature of several dilute magnetic semiconductor (DMS) materials can be predicted quite accurately by using the local-density approximation (LDA) electronic structure calculations and Monte Carlo simulations (MCS). The calculations based on this framework, however, do not predict the high-Curie-temperature ferromagnetism in wide-gap DMS, such as ZnO- and GaN-based systems [1]. According to the theory, due to the short-rangeness of the magnetic exchange interaction, it is impossible to form magnetic percolation path in the materials. In this paper, for the purpose to explain the ferromagnetic behavior of ZnO-based DMS at high temperature in experiments [2], we propose the possibility of formation of the spinodal decomposition (SD) phase in ZnO-based DMS. It has been proposed that in the SD phase of Mn-doped GaN [3] and Cr-doped ZnTe[4], the local fluc-tuation in concentration of the magnetic impurities would support the magnetic network. To verify this possibility, we perform computer simulations for the SD phase formation in ZnO-based DMS. Our simulation method consists of three steps. Firstly, we calculate the electronic structure of ZnO-based DMS by using the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method [5] and evaluate chemical pair interactions between magnetic impurities in ZnO. Then we simulate the formation of the SD phase by performing MCS on an Ising-type model which describes the distribution of the impurities. Finally, we estimate Curie temperature of the SD phase and compare it with Curie temperature of the homogeneous phase in order to discuss the effect of the formation of the SD phase.

[1] L. Bergqvist et al., Phys. Rev. Lett. 93 (2004) 137202; K. Sato et al., Phys. Rev. B 70 (2004) 201202.
[2] H. Saeki et al., Solid State Commun. 120 (2000) 439; K. Ueda et al., Appl. Phys. Lett. 79 (2001) 988; K. Rode et al., J. Appl. Phys. 93 (2003) 7676.
[3] K. Sato et al., Jpn. J. Appl. Phys. 44 (2005) L948.
[4] T. Fukushima et al., Jpn. J. Appl. Phys. 45 (2006) L416.
[5] H. Akai and P. H. Dederichs, Phys. Rev. B 47 (1993) 8739.

Relativistic treatment of spin currents and spin-transfer torques

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It will be shown that a useful relativistic generalization of the conventional spin density s(r,t) for the case of moving electrons is the expectation value (?(r,t),?4(r,t)) of the four-component Bargmann-Wigner polarization operator T?=(T,T4) with respect to the four component Dirac wave function ? (r,t). An exact equation of motion for this quantity is derived, using the one-particle Dirac equation, and the relativistic analogues of the non-relativistic concepts of spin-currents and spin-transfer torques are identified. In the classical limit the time evolution of (?,?4), the integral of (?(r,t),?4(r,t)) over the volume of a wave packet, is governed by the equation of motion first proposed by Bargmann, Michel and Telegdi (prl 2, 435, 58 see also L+L Vol.4 Quantum Electrodynamics) generalized to the case of inhomogeneous systems. In the non-relativistic limit it is found that the spin-current has an intrinsic spin-Hall contribution and to order 1/c? a spin-orbit coupling related torque appears in the equation of motion for ?(r,t). The relevance of these results to the theory of the intrinsic spin Hall effect and current-induced switching will be briefly discussed.

Noncollinear magnetism within OEP view to spindynamics

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The dynamics of the spin degree of freedom is responsible for phenomena like spin injection and spin filtering. These mechanisms are crucial for recent developments in e.g. spintronics and spin transport. The advent of the time dependent extension of SDFT has made the ab-initio treatment of spin dynamics possible. Crucial to practical calculations using SDFT is the approximation made for the exchange-correlation energy functional. In calculations this has most often been approximated with the LSDA, GGA or the corresponding time dependent extensions. These have been developed for collinear magnetism, and their use in non-collinear situations relies on the magnetisation (m(r)) and exchange correlation magnetic field (B_{xc}(r)) being made collinear in a local reference frame at each point in space and at each time. Under such an approximation m(r) x B_{xc}(r) vanishes everywhere in space. This renders all such calculations unsuitable for ab-initio spin dynamics in the adiabatic approximation, a serious limitation of these functionals. In this conference I will talk about the generalization of OEP formalism for SDFT to non-collinear magnetic systems. Crucially, I do not rely on a condition of local collinearity. Using the exact exchange (EXX) functional and with the example of an unsupported Cr(111) monolayer, I will show that in general magnetisation and B_{xc}(r) are

not parallel - in contrast to what is usually assumed in all to date non-collinear calculations. This renders the TD extensions of EXX functional suitable for the study of dynamical spin effects.

Spiral magnetic structures driven by spin-orbit coupling: Determining the Dzyaloshinsky vector from first principles

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In certain crystal symmetries (in particular at surfaces), spin-orbit coupling can give rise to an antisymmetric exchange interaction, known as Dzyaloshinsky-Moriya interaction (DMI). In magnetic systems, this interaction favors spatially rotating spin structures of a certain rotational direction. In order to know, whether the DMI is strong enough to compete with the spin stiffness and anisotropy energy, we compare the electronic energies of spin spirals of opposite rotational directions. For this, we present a computational scheme that allows to estimate the energies of spin spirals with long spatial periods from first principles. Thereby, we treat the spin-orbit coupling as a perturbation to homogeneous spin spirals that are obtained with a scalar-relativistic Hamiltonian. The latter spirals are calculated within the chemical unit cell by using a generalized Bloch theorem [Sandratskii, phys.stat.sol. (b) 135, 167 (1986)]. We apply our method to two systems: (i) a monoatomic Mn film deposited on the W(110) surface which shows on top of the local antiferromagnetic structure a long-ranged modulation caused by the DMI, (ii) a similar system, namely two atomic layers of Fe on W(110), where the DMI is strong enough to influence the orientation of the domain walls. In both cases, we investigate the magnetic structure with a micromagnetic model and obtain the corresponding model parameters from ab-initio calculations. Our theoretical results compare nicely with recent STM experiments [e.g. Bode et. al., PRL 89, 237205 (2002); Vedmedenko et. al., PRL 92, 077207 (2004)].

Ab-initio ballistic conductance with spin-orbit coupling

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Ballistic conductance ab-initio calculations in heavy metal break junctions require a very accurate description of the nanocontact electronic structure near the Fermi level, in turn quite sensitive to relativistic effects and particularly to spin-orbit coupling. The complex k-vector approach proposed by Choi and Ihm [1] for calculating the ballistic conductance of open quantum systems within the

Landauer-Buttiker approach is generalized to the recently introduced fully relativistic ultrasoft pseudo-potentials [2] in order to deal with ballistic transport in presence of spin-orbit coupling. We present applications of the above formalism to the electronic structure, magnetic properties, and ballistic electron transport in infinite monatomic Pt nanowires [3] and in a short nanowire contact between two tips. We compare the fully relativistic and the scalar relativistic results, highlighting the net effect of spin orbit.

[1] H. J. Choi and J. Ihm, Phys. Rev. B 59, 2267 (1999); A. Smogunov, A. Dal Corso, and E. Tosatti, Phys. Rev. B 70, 045417 (2004).

[2] A. Dal Corso and A. Mosca Conte, Phys. Rev. B 71, 115106 (2005).

[3] A. Dal Corso, A. Smogunov, and E. Tosatti, Phis. Rev. B, to appear.

The nature of the unusual sequence of phase transitions in MnAs: The first-principles study

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Manganese Arsenide attracts much research attention by an unusual combination of physical properties. At 313 K MnAs experience a first order phase transition. Both atomic structure and the magnetic state are changed discontinuously. The lattice transforms from hexagonal NiAs to orthorhombic MnP type. Simultaneously, the ferromagnetism of the system disappears. Because of controversial experimental properties the nature of the magnetic state above the first phase transition is still the matter of debate. It can be classified neither as antiferromagnet or as paramagnet. At 400 K, a second-oder phase transition takes place. The lattice returns back to the NiAs type whereas the magnetic state becomes a usual Curie-Weiss paramagnetism. Among other interesting properties of the system are the similarity of the magnetoresistance properties to the colossal magnetoresistance in Mn perovskites and a strong magneto-caloric effect useful for magnetic refrigeration. I will report on the first first-principles study of the exchange interactions and magnetic transition temperature in MnAs. An interpretation of the phase transitions is suggested. Besides the properties of the particular system some general questions will be addressed: the quality of the mapping on the Heisenberg model for compounds with well-defined atomic moments, the noncollinearity of the magnetic structure governed by the properties of the induced magnetic moments of anions.

Calculation of magnetic interactions in Cr spinels

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Effective exchange coupling constants between Cr spins in ACr_2X_4 (A=Zn, Cd; X=O, S, Se) spinels are estimated by mapping the energy of spin spirals

calculated within LSDA and LSDA+U approximations onto an effective Heisenberg model. The calculations reproduce the change of the sign of the exchange coupling between nearest Cr neighbours from anti-ferromagnetic (AFM) in O-based spinels to ferromagnetic (FM) in S and Se based ones. It is shown that the AF nearest neighbour coupling in ACr2O4 is determined mainly by direct hopping between Cr t2g electrons whereas the FM coupling S(Se)-based spinels is caused by Cr t_{2g}-X p-Cr t eg hybridization.

Competing interactions in the low-dimensional quantum magnet TiOCl

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The layered quantum spin system TiOCl, a Mott-Hubbard insulator, has created significant amount of interest in recent years because of its anomalous behavior manifested in susceptibility measurements, ESR, Raman spectroscopy and photoemission experiments. We have studied the electronic and magnetic properties of this system [1,2,3,4] by means of density functional calculations and have investigated the possible effects of spin, phonon and orbital degrees of freedom and conclude that frustration plays an important role in the behavior of this system. Here we will present an overview.

[1] T. Saha-Dasgupta, R. Valenti, H. Rosner, C. Gros, Europhys. Lett. 67 63 (2004).

[2] T. Saha-Dasgupta, A. Lichtenstein, R. Valenti, Phys. Rev. B 71, 153108 (2005).

[3] L. Pisani, R. Valenti, Phys. Rev. B (RC) 71, 180409 (2005).

[4] M. Hoinkis, M. Sing, J. Schaefer, M. Klemm, S. Horn, H. Benthien, E. Jeckelmann, T. Saha-Dasgupta, L. Pisani, R. Valenti, R. Claessen, Phys. Rev. B 72, 125127 (2005).

Complex magnetic order and transition to half-metallicity in Mn-doped Fe_3Si

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Fe_3Si is a ferromagnetic material with possible applications in magnetic tunnel junctions [1]. When doped with Mn, the material shows a complex magnetic behavior, as suggested by older experiments [2]. Motivated by the above, we employed the Korringa-Kohn-Rostoker Green function method within density-functional theory in order to study the alloy $Fe_{3-x}Mn_xSi$, with $0<x<1$ The Mn atoms are positioned at the octahedral site of the $L2_1$ crystal structure. Chemical disorder is described within the coherent potential approximation (CPA).

Using the generalised gradient approximation (GGA) of density-functional theory, we find that the Mn moments are ferromagnetically aligned to the Fe moments for all concentrations 0 ¡ x 1, in accordance with experimental findings [2]. In contrast to this, the local density approximation (LDA) gives a (wrong) antiferromagnetic Mn-Fe coupling for low concentrations. As the Mn concentration increases, the spin polarization P at the Fermi level changes drastically, from negative values for the clean Fe3Si (P(x=0)=-0.3), to high positive values (e.g., P(x=0.6)=0.96). For x=1 the system becomes half-metallic (P=1). At the same time, the Curie temperature drops from T_C = 823 K (x=0) to T_C =214 K (x=1). This is reflected in the values of the exchange constants. At intermediate concentrations, high polarization coexists with high TC, suggesting applicability in spintronics. Finally, we discuss an anomaly in the magnetization curve M(T)observed experimentally [2] for x¿0.75.

[1] A. Ionescu et al., Phys. Rev. B 71 , 094401 (2005)

[2] S. Yoon and J. G. Booth, J. Phys. F: Met. Phys. 7, 1079 (1977)

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