

Report on "Computational Magnetism and Spintronics 2010" Workshop

Bonn, Gustav-Stresemann-Institut, Germany

May 10th-12th 2010

Psi-k Network and Forschungszentrum Jülich

Stefan Blügel and Yuriy Mokrousov (Forschungszentrum Jülich)

Alexander Shick (Institute of Physics, ASCR, Prague)

<http://www.fz-juelich.de/iff/CompMag2010/>

Scientific Report

Spintronics, magnetoelectronics and magnetism continues to be very creative, innovative and active research themes in condensed matter physics. The Hall effects, the concept of topological matter, the Dzyaloshinskii-Moriya interaction in inversion symmetry broken solids, the magnetoelectric coupling, the spin-transfer torque, magnetic susceptibilities, multiferroicity at oxide interfaces and heterostructures are issues which emerged during the past 5 years and represent vital scientific issues of broad scientific and technological interest. These fields are progressing very fast and continue branching into increasingly wider areas of condensed matter: these include the strongly correlated electron systems, multiferroic oxides and oxide junctions, oxides and semiconductors in terms of diluted magnetic semiconductors, to organic and inorganic molecules in terms of molecular magnets, and carbon nanotubes in the field of nano-spintronics or even to ferroelectric materials in terms of multiferroics. Moreover, it is widely recognized that first-principles calculations on magnetic materials can give important clues to understanding properties and behavior of different materials and can have a remarkable impact both from the basic as well as from the technological point of view.

However, within the rich and vivid field of magnetism, there are few opportunities to discuss – within the *ab-initio* community – issues such as accuracy and limits of density functional theory for novel magnetic materials, methods development, specific computational issues, etc. This motivated in 2006 the working groups Magnetoelectronics and Complex Magnetism of the Psi-k Network to organize within the next years a regular series of conferences and workshops, which will be integrated within the new cooperation between Psi-k and CECAM (Centre European de Calcul Atomique et Moléculaire). Every second year it is planned to have a conference with maximum 60 participants on a broader scope of content and every other year we think of a more focused Psi-k/CECAM-workshop (or two of them). In 2008, O. Eriksson, I. Mertig, and P. Zahn organized the CCMS08 in Dresden. The current workshop was in the line of such meetings.

In the workshop "Computational Magnetism and Spintronics 2010" we tried to bring together leading experts in first-principles description of magnetic properties, spin excitations, spin-orbit interaction, spin dynamics and spin-dependent transport in solids and nanostructures. This year we focussed on (i) recent developments in spin-orbit related phenomena due to symmetry breaking on surfaces and interfaces, skyrmion lattice, Dzyaloshinskii-Moriya interaction (G. Bihlmayer), (ii) spin-orbit interaction-driven

transport properties such as anisotropic magnetoresistance, anomalous Hall and spin Hall effects (I. Turek, H. Ebert, F. Freimuth), (iii) spin-relaxation and spin-torque (M. Stiles, Z. Yuan, A. Starikov), (iv) magnetoelectric coupling (C. Ederer, A. Ernst), (v) spin-dependent transport (A. Smogunov, S. Khmelevskiy, C. Heiliger), (vi) developments beyond LDA (P. Rinke, L. Nordström, M. Schlipf), (vii) multiferroics, oxides, oxide interfaces (M. Stengel, R. Pentcheva, S. Picozzi, I. Popov), (viii) spin dynamics and spin excitations (A. Schindlmayr, L. Sandratskii, L. Nordström, M. Katsnelson, R. Muniz, A. Pertsova), (ix) electron paramagnetic resonance (U. Gerstmann). Each presentation of the workshop was followed by intensive discussions among the participants of the workshop. The general scientific atmosphere of the discussions and the workshop in general was open and creative.

Program

Monday, May 10th 2010

9:00–9:20 Stefan Blügel: Welcome

9:20–10:00 Gustav Bihlmayer: "Two-dimensionally modulated spin-structures at surfaces"

10:00–10:40 Silvia Picozzi: "Electronic magnetic ferroelectrics: modelling and understanding"

10:40–11:00 Coffee break

11:10–11:50 Claude Ederer: "Different ways to couple magnetism and electric polarization in multiferroic materials"

11:50–12:30 Patrick Rinke: "Approaching unity: the advanced DFT functionals exact-exchange and RPA meet quasiparticle energy calculations"

12:30–14:30 Lunch break

14:30–15:10 Lars Nordström: "Polarizations of transition metals: the role of higher multipoles - hidden orders and complex magnetism"

15:10–15:30 Igor Popov: "Multiferroicity of magnetism hexaboride"

15:30–16:00 Martin Schlipf: "Hybrid Functionals within the All-Electron FLAPW Method: Implementation and Applications"

16:00–16:30 Coffee break

16:30–17:10 Mikhail Katsnelson: "Towards *ab initio* spin dynamics"

17:10–17:50 Lars Nordström: "Atomistic spin dynamics: recent progress"

18:00–22:00 Poster session

Tuesday, May 11th 2010

9:00–9:40 Hubert Ebert: "Ab initio investigation of the Spin Hall Effect for non-magnetic alloys"

9:40–10:20 Ilja Turek: "Anisotropic magnetoresistance and anomalous Hall effect in random ferromagnetic alloys"

10:20–10:40 Frank Freimuth: "Orientational dependence of the spin-Hall conductivity: toy models and first-principles calculation"

10:40–11:10 Coffee break

11:10–11:50 Arthur Ernst: "Magneto-electric coupling in thin films"

11:50–12:30 Rossitza Pentcheva: "Tayloring Electronic States at Oxide Surfaces and Interfaces"
12:30–12:50 Hubert Ebert: "Orbital-dependent functionals within the KKR-multiple scattering formalism - an implementation of exact exchange"
12:50–14:30 Lunch break
14:30–15:10 Sergii Khmelevskiy: "Spin-orbit coupling induced anisotropy effects and exchange interactions in Mn-based bimetallic antiferromagnets"
15:10–15:50 Alexander Smogunov: "Locally magnetic nanostructures: interplay between magnetism and electron transport"
15:50–16:10 Christian Heiliger: "Calculations of spin dependent transport in MnAs"
16:10–16:40 Coffee break
16:40–17:20 Roberto Muniz: "Spin dynamics in magnetic metallic nanostructures"
17:20–18:00 Leonid Sandratskii: "Non-adiabatic spin-dynamics of complex magnetic systems"
18:00–18:20 Anna Pertsova: "Dynamics of localized spin impurities in one-dimensional wires"
19:00–22:00 Conference dinner

Wednesday, May 12th 2010

9:00–9:40 Arno Schindlmayr: "Spin excitations in itinerant ferromagnets from first principles"
09:40–10:20 Mark Stiles: "Calculation of spin-orbit induced relaxation in transition metal ferromagnets"
10:20–10:40 Anton Starikov: "A first-principles study of the resistivity, Gilbert damping and spin-flip diffusion in $\text{Ni}_{1-x}\text{Fe}_x$ substitutional alloys"
10:40–11:10 Coffee break
11:10–11:30 Zhe Yuan: "Non-adiabatic spin torque in magnetic domain walls from first principles"
11:30–12:10 Massimiliano Stengel: "Proper treatment of the macroscopic variables in multi-ferroic systems"
12:10–12:50 Uwe Gerstmann: "Magnetic properties of surface and interface states investigated via ab initio g-tensor calculations"
12:50 - 14:30 Lunch Break

List of participants

Mikhail Katsnelson (Radboud University Nijmegen, The Netherlands)
Leonid Sandratskii (Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany)
Claude Ederer (School of Physics, Trinity College, Dublin, Ireland)
Roberto Muniz (Universidade Federal Fluminense, Niteroi, Brazil)
Lars Nordström (Department of Physics, Uppsala University, Sweden)
Arthur Ernst (Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany)
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Two-dimensionally modulated spin-structures at surfaces

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Prototypical magnetic structures at surfaces are spiral spin-density waves (SSDWs) or collinear structures which can be regarded as special SSDWs. The formation of SSDWs can be driven e.g. by magnetic frustration [1] or the Dzyaloshinskii-Moriya (DM) interaction [2]. Higher order magnetic interactions, like the four-spin interaction, can couple spin-spirals to form two-dimensionally modulated structures in special cases [3]. In combination with a strong DM term, unique magnetic structures – so called Skyrmions – can form in ultrathin films on heavy substrates. The special topology of these structures can enhance the stability of otherwise fragile magnetic structures, as can be observed for a monolayer of iron on an Ir(111) substrate [4]. Density functional theory calculations show that the strengths of the different magnetic interactions (Heisenberg-type exchange, DM- and four-spin interaction, magnetic anisotropy) are in the right range to allow for a nanoskyrmion lattice as a ground state. This complex magnetic structure is also observed experimentally by scanning tunneling microscopy in spin-polarised mode and spin-orbit contrast [5].

[1] B. Hardrat, A. Al-Zubi, P. Ferriani et al., Phys. Rev. B **79**, 094411 (2009).

[2] M. Bode, M. Heide, K. von Bergmann et al., Nature **447**, 190 (2007).

[3] Ph. Kurz, G. Bihlmayer, K. Hirai, and S. Blügel, Phys. Rev. Lett. **86**, 1106 (2001).

[4] S. Heinze, K. von Bergmann, M. Menzel, A. Kubetzka, R. Wiesendanger,

G. Bihlmayer and S. Blügel (submitted).

[5] M. Bode, S. Heinze, A. Kubetzka et al., Phys. Rev. Lett. **89**, 237025 (2002).

CALCULATIONS OF SPIN DEPENDENT TRANSPORT IN MnAs

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Magnetic MnAs nanoclusters can be grown on a GaAs substrate in a controlled manner [1]. Such structures can be used to construct planar magnetic devices for spintronic applications. We perform *ab initio* calculations by means of the non-equilibrium Keldysh formalism implemented in the Korringa-Kohn-Rostoker Green's function method [2]. We study the spin-dependent transport of MnAs in the hexagonal NiAs structure along different crystallographic directions. Furthermore we discuss in detail the transport through interfaces formed by two MnAs clusters with different magnetic domains. We found a very large magnetoresistance ratio above 200% while the spin polarization is low, which is originated by the different Fermi surface topologies of the two spin channels.

[1] S. Ito, S. Hara, T. Wakatsuki and T. Fukui, Appl. Phys. Lett. 94, 243117 (2009)

[2] C. Heiliger, M. Czerner, B. Yu. Yavorsky, I. Mertig, M. D. Stiles, J. Appl. Phys. 103, 07A709 (2008)

Ab initio investigation of the Spin Hall Effect for non-magnetic alloys

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Spin-orbit coupling is responsible for several interesting phenomena like e.g. the anomalous Hall effect (AHE) in magnetic materials. The AHE results from the interaction between spin-orbit coupling and the spin polarization. In comparison to the AHE the spin Hall effect (SHE) needs no spin polarization and is therefore even present in non-magnetic systems. This was shown by several experimental works e.g. [1,2]. During the last years several publications have appeared which studied the spin Hall effect for pure systems via *ab initio* [3,4] or model calculations [5]. However, up to now no publication is available in which the SHE is calculated for alloy systems on an *ab initio* level. To calculate the SHE we have implemented the Kubo-Středa equation in our fully relativistic SPR-KKR package. The Kubo-Středa equation gives access to the full anti-symmetric conductivity tensor what is necessary for the calculation of the SHE. The disorder is treated via the coherent potential approximation (CPA). We show first results for several non-magnetic *3d* and *4d* transition metal alloys.

[1] S. O. Valenzuela and M. Tinkham, Nature **442**, 176 (2006)

[2] T. Kimura, et al. , Phys. Rev. Lett. **98**, 156601 (2007)

[3] Y. Yao and Z. Fang, Phys. Rev. Lett. **95**, 156601 (2005)

[4] G. Y. Guo, S. Murakami, T.-W. Chen and N. Nagaosa, Phys. Rev. Lett. **100**, 096401 (2008)

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DIFFERENT WAYS TO COUPLE MAGNETISM AND ELECTRIC POLARIZATION IN MULTIFERROIC MATERIALS

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In this talk I will discuss how first principles calculations using density functional theory can be used to explore different ways to couple magnetism and electric polarization in multiferroic materials.

Note: Full abstract will be provided later.

Atomistic Spindynamics; recent progress

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Recent developments in atomistic spin-dynamics are presented, both methodologically as well as applications with materials specific parameters. Examples will be presented from thin-film magnetism, diluted magnetic semi-conductors as well as for devices used for ultra-fast switching phenomena.

Note: Abstract submission deadline is **March 1, 2010**

Magneto-electric coupling in thin films

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In my talk I shall discuss several aspects of magneto-electric coupling in thin films. In these systems, the presence of a surface can change structural, electronic and magnetic properties of composite materials thereby modifying significantly magneto-electric coupling in addition to interface effects. In the first part of my talk I shall present our first-principles calculations of ultrathin Fe films deposited on TiO₂-terminated (001) surfaces of BaTiO₃ perovskite, which exhibit an unexpected change in their magnetic structure with increasing Fe-film thickness. Furthermore, I'll demonstrate how these properties can be manipulated by alloying the Fe films with other 3d transition metals. In the second part of my talk, I'll discuss magneto-electric coupling in pure metallic systems. In metals an external electric field is screened up on the surface by free electric charges. Nevertheless, the electric field can strongly interact with the induced surface charge. Under an applied electric field this induced surface charge can experience strong vertical displacements according to the sign of the applied field. In its turn, the screening charge exerts forces on the atomic nuclei, which cause relaxations of their positions in vicinity of the surface. In magnetic systems these processes can lead to alteration of the magnetic ordering. I'll discuss these effects on example of two atomic layers of Fe grown on Cu(111), studied with a first-principles approach and scanning tunneling microscopy experiments.

Orientalional dependence of the spin-Hall conductivity:

Toy models and first-principles calculations

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The spin-Hall effect (SHE) and the anomalous Hall effect (AHE) have the same origin: The spin-orbit interaction gives rise to a spin-dependent force on the electrons. In the case of the AHE it is known [1] that the associated conductivity is dependent on the magnetization direction. Based on first-principles calculations we predict that the SHE exhibits a similar orientational dependence in non-cubic geometries. However, in contrast to the AHE, this effect is of purely geometrical origin. Our calculations were performed using the full-potential linearized augmented-plane-wave (FLAPW) method FLEUR (www.flapw.de) and maximally localized Wannier functions [2] as an efficient basis set. For a simple three-band model we investigate how the anisotropy of the conductivity is related to hoppings and the spin-orbit coupling matrix.

References

- [1] Eric Roman, Yuriy Mokrousov, and Ivo Souza *Orientation Dependence of the Intrinsic Anomalous Hall Effect in hcp Cobalt*, Physical Review Letters, **103**, 097203 (2009)
- [2] F. Freimuth, Y. Mokrousov, D. Wortmann, S. Heinze and S. Blügel, *Maximally localized Wannier functions within the FLAPW formalism*, Physical Review B, **78**,035120 (2008),
I. Souza, N. Marzari, and D. Vanderbilt *Maximally localized Wannier functions for entangled energy bands*, Physical Review B, **65**, 035109 (2001)

Magnetic properties of surface and interface states investigated via *ab initio* g -tensor calculations

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Electron paramagnetic resonance (EPR) provides a powerful tool to analyse the microscopic structure of paramagnetic systems. For defects in semiconductors, this is well known and frequently used since several decades. Here, we show that the EPR parameters of surface and interface structures are exceptionally sensitive quantities which help to elucidate the magnetic properties of the microscopic structures. Hydrogenated microcrystalline silicon ($\mu\text{c-Si:H}$) provides a very interesting example. The material can be used for efficient and low-cost solar cells whereby the porosity of this material allows in-diffusion of atmospheric gases. The main effects to consider are oxidation and adsorption of hydrogen on surfaces.

In this work, we characterize the magnetic properties of the resulting surface states by calculating the electronic g -tensors from first principles using the gauge-including projector augmented plane wave (GI-PAW) approach [1, 2] in the framework of density functional theory. We find that hydrogen adsorption at the Si surfaces influences the magnetic signature of the material dramatically, whereby a large variety of g -tensors is obtained. The influence of oxidation, in contrast, is surprisingly small. The g -tensors resemble those of the corresponding hydrogenated surfaces, suggesting that the spin-orbit coupling and, by this, the magnetic properties of the Si/SiO₂ interface are predominantly influenced by the crystalline part of the structures.

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[2] U. Gerstmann, M. Rohrmüller, F. Mauri, W.G. Schmidt, *phys. stat. sol. (c)* **7**, 157 (2010).

Towards *ab initio* spin dynamics

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I review basic approaches which can be used to deal with spin dynamics and related properties in completely *ab initio* way. First, a general expression for the dynamic susceptibility in the framework of time-dependent density functional is discussed, as well as its simplifications in adiabatic and local density approximations. Several ways to derive first-principle exchange parameters are presented and compared, both within the density functional and beyond (LDA+U, LDA+DMFT). Applications to magnetic transition metals and molecular magnets are chosen as examples of the general scheme. An *ab initio* approach to calculate relativistic magnetic interactions, in particular, Dzialoshinski – Moriya parameters, is considered.

**SPIN-ORBIT COUPLING INDUCED ANISOTROPY EFFECTS AND
EXCHANGE INTERACTIONS IN Mn-BASED BIMETALLIC
ANTIFERROMAGNETS.**

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The magnetic anisotropy and exchange interactions in 3d-5(4)d Mn-based AFM's are studied in the framework of the density functional theory. The magnetic force theorem and the torque method are used to obtain the atom-resolved contributions to the MAE. For MnX (X=Pt,Pd,Rh) we found a competition between Mn- and 5(4)-d-element contributions into the MAE. The MAE is substantially enhanced in MnIr, where the Ir-atom contribution dominates over a weak Mn-atom MAE. The Neel temperatures have been calculated using Monte-Carlo method and essential differences in the exchange interactions in AF ground state and DLM state are found. The large strain dependent anisotropy in DOS in MnIr and Mn₂Au is identified. We propose the new concept of using these materials in spintronics applications.

Orbital-dependent functionals within the KKR-multiple scattering formalism - an implementation of exact exchange

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We present the formalism and implementation of a relativistic optimized effective potential method in the framework of exact exchange (EXX) within spin-DFT. All ingredients of the integral equation are expressed in terms of the KKR-GF, thereby avoiding a basis set formulation. The real-space static Kohn-Sham response function as well as the inhomogeneity of the integral equation are expressed in terms of the GF. In the all-electron formulation, core, valence and their respective cross terms are treated explicitly. By imposing appropriate boundary conditions the associated core part of the code can be used to calculate free (open-shell) atoms. [1,2] A formulation of the RPA within the scheme is sketched. We further give examples of the application of the method to solids using EXX. [3]

Literature:

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- [2] E Engel, D Ködderitzsch, H Ebert, Phys. Rev. **B 78**, 235123 (2008)
- [3] D Ködderitzsch, H Ebert, H Akai, E Engel, J. Phys: Condens. Matter, **21**, 064208 (2009)

SPIN DYNAMICS IN MAGNETIC METALLIC NANOSTRUCTURES

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Theoretical studies on spin dynamics in magnetic metallic nanostructures are presented. The nature and characteristics of the spin-wave excitations in ultrathin ferromagnetic films adsorbed on semi-infinite non-magnetic metallic substrates are investigated. The spin wave spectra, including their dispersion relations and linewidths, are calculated throughout the surface Brillouin zone, for various films with different thicknesses, and substrate combinations. Our results are compared with experimental Spin Polarized Electron Energy Loss Spectroscopy (SPEELS) data, and also with theoretical predictions based on the adiabatic description of spin motions. We show that the description of spin waves based on the adiabatic approximation breaks down qualitatively in all the systems we have studied, because it overlooks Landau damping, which is appreciable at shorter wavelengths. Our dynamical theory produces a single very broad feature in the spectral density at large wave vectors, in very good agreement with what is observed in SPEELS experiments. Results for Fe monolayer and bilayer over W(110) surface are examined, and the importance of the substrate to the electronic structure and to spin-wave spectra is discussed. We conclude by exploring effects of the spin-orbit coupling on the spin-wave excitations.

Polarizations of transition metals: the role of higher multipoles – hidden orders and complex magnetism.

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The concept of polarizations of an open atomic shell is reviewed and discussed. Especially it is presented how this discussion become simple and beautiful in terms of the so-called spherical tensor moments or spherical multipoles. Some of these multipoles are already known to play an important role in e.g. x-ray circular dichroism measurements, where with the use of the famous sum rules by Carra et al. the spin and orbital magnetic moments can be deduced.

Here we will describe how such multipoles can be calculated in general in both the ground state as well as excited states in terms of density functional methods including a local correlation term, as in e.g. the so-called LDA+U or LDA+DMFT methods. It will be demonstrated how these multipoles can contribute significantly to the exchange and correlation energies of transition metal systems.

For systems where the spin-orbit coupling is significant, our results are in fair agreement with experiments but the calculated polarizations do not follow Hund's rules. This lead us to suggest an alternative set of rules, Katt's rules, that better describe our results.

We will discuss in some depth materials where these multipoles act as the main order parameter, often referred to as an "hidden order". Results will be presented for the heavy fermion compound URu₂Si₂, the insulator NpO₂ and the magnetic/superconducting iron-pnictide LaOFeAs.

Tayloring Electronic States at Oxide Surfaces and Interfaces

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The polar discontinuity in oxide heterostructures and thin films can lead to novel electronic states even when simple band insulators as LaAlO_3 and SrTiO_3 are involved. Density functional theory calculations show that a strong lattice polarization allows several layers of LaAlO_3 to remain insulating before an electronic reconstruction takes place at around 4 MLs [1]. Here we demonstrate that a capping STO layer can trigger the insulator-to-metal transition already at two MLs of LaAlO_3 . As a result two spatially separated sheets of carriers emerge: electrons at the interface and holes at the surface, that are only 1 nm apart.[2]

In the second part of my talk I will address the adsorption of water molecules on the $\text{Fe}_3\text{O}_4(001)$ surface and how they influence the surface reconstruction and the charge and orbital order of magnetite(001) [3].

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2. R. Pentcheva, M. Huijben, K. Otte, W.E. Pickett, J.E. Kleibecker, J. Huijben, H. Boschker, D. Kockmann, W. Siemons, G. Koster, H.J.W. Zandvliet, G. Rijnders, D.H.A. Blank, H. Hilgenkamp, and A. Brinkman, *Phys. Rev.Lett*, in press; cond-mat/0912.4671.
3. N. Mulakaluri, R. Pentcheva, M.Wieland, W. Moritz and M. Scheffler, *Phys. Rev. Lett.* **103**, 176102 (2009).

DYNAMICS OF LOCALIZED SPIN IMPURITIES IN ONE-DIMENSIONAL WIRES

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Low-dimensional atomic-scale magnetic structures represent a rich playground for spin-dynamic phenomena. Along with remarkable experimental advances in such fields as single spin manipulation [1], there is an increased interest in theoretical investigations and modelling of spin dynamics at the atomic scale.

In this work, we adopt a mixed quantum-classical theoretical description to study the spin-dynamics in atomic structures, which is based on the Ehrenfest scheme [2]. The model system consists of one or several localized spins implanted in a one-dimensional atomic wire. Our time-dependent simulations demonstrate how a spin-excitation, produced over one of the localized spins, is propagated by the itinerant electrons along the wire, forming a complex pattern of spin-density excitations.

One problem that we are addressing within this framework is how an electrostatic gate can tune the effect of a spin-excitation in the wire coupling two spin impurities. We address this issue by analyzing the dynamical spectrum of the system and its dependence on the internal parameters, defining the electronic structure and external perturbation (such as the applied electrostatic gate).

References: [1] R. Hanson *et al.*, Nat. 453, 1043 (2008) [2] M. Stamenova and S. Sanvito in The Oxford Handbook of Nanoscience and Technology, Vol. 1, Oxford University Press (2010).

ELECTRONIC MAGNETIC FERROELECTRICS: MODELLING AND UNDERSTANDING

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The coexistence of long-range dipolar and magnetic orders occurs in the so-called *multiferroics*, one the most interesting examples of multifunctional compounds in modern materials science. In particular, *electronic magnetic ferroelectrics*, i.e. complex magnetic oxides in which ferroelectricity is driven by non-centrosymmetric spin- or charge- or orbital-arrangements, have recently attracted great interests. By means of density functional studies, we will focus on the existence and efficiency of different mechanisms for multiferroicity, based on the interplay between electronic and structural degrees of freedom.[1]

In closer detail, we will present cases in which a magnetically-induced electric polarization is driven by symmetric (Heisenberg-like) exchange interactions, at variance with well-known examples (such as spiral-like TbMnO_3), in which the polarization is induced by antisymmetric (Dzyaloshinskii-Moriya-like) exchange. Examples include orthomanganites, nickelates (LuNiO_3 , HoNiO_3), sulfides (such as $\text{Cu}_2\text{MnSnS}_4$) and orthoferrites.

The second part of our presentation will be devoted to the possibility of achieving ferroelectricity induced by a non-centrosymmetric charge-order. For example, ferrimagnetic Fe_3O_4 below the Verwey transition shows an electric polarization of few $\mu\text{C}/\text{cm}^2$, induced by a charge-ordered pattern of $\text{Fe}^{2+}/\text{Fe}^{3+}$ on the Fe B sites of the inverse spinel structure.

Finally, we will present promising avenues towards other examples where charge-ordering or spin-ordering or a combination of both spin-and-charge-ordering driven ferroelectricity can occur, in terms of novel materials, unconventional mechanisms and related efficiency.

[1] For further info, please see <http://www.casti.aquila.infn.it/homepages/bismuth/index.html>

MULTIFERROICITY OF MAGNESIUM HEXABORIDE

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Hexaborides, MB_6 ($M=Ca, Sr, Ba$), have attracted considerable attention after the observation of a weak ferromagnetism not involving partially filled d or f orbitals. High melting point, chemical stability and high hardness are among other properties which raised the interest in these compounds. Although the above mentioned systems were thoroughly investigated theoretically and experimentally, the properties of the lighter member of the family, namely MgB_6 , are largely unknown so far.

Our spin-polarized calculations, based on DFT at GGA level, predict multiferroicity in MgB_6 , which is unique in this class of materials. In fact, MgB_6 displays a weak magnetic moment associated to boron vacancies, similar to the ferromagnetism in the related CaB_6 and SrB_6 . In addition, a small Mg cations shift off the center of the simple cubic elementary unit cell breaks the central symmetry and yields the relatively large net electric dipole moment of 7.7 Debye per unit cell. Long range Coulombic interaction lowers the energy of the system further by arranging the dipoles in antiferroelectric order.

Note: Abstract submission deadline is **April 1, 2010**.

Approaching unity: the advanced DFT functionals Exact-Exchange and RPA meet Quasiparticle Energy Calculations

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Local- and semilocal density approximations (LDA/GGA) to density functional theory (DFT), although tremendously successful in electronic structure calculations, are cursed by severe self-interaction errors. These can lead to qualitative failures, as exemplified by the “CO adsorption puzzle” where LDA and GGA predict the wrong adsorption site for a CO molecule on (111) surfaces of Cu, Rh, and Pt [1] or semiconductors like InN, ScN, [2], FeO, CoO [3] or the lanthanide sesquioxides [4] for which LDA and GGA predict a metallic behaviour. I will show that removing the self-interaction error in DFT by means of the exact-exchange optimized effective potential approach (OEPx) turns these materials into semiconductors [2,3]. The OEPx ground state then provides a suitable starting point for quasiparticle energy calculations in the G_0W_0 approximation [2]. Going beyond OEPx in DFT, a physically motivated correlation energy *en par* with the GW self-energy can be achieved in the random phase approximation (RPA). I will discuss the current state-of-the-art in RPA and demonstrate that it recovers the correct (on-top) adsorption site for CO@Cu(111) [1].

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Non-adiabatic spin-dynamics of complex magnetic systems

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We report parameter-free calculation of the transversal dynamic susceptibility in a number of complex magnetic systems. This theoretical approach accounts on an equal footing for both single-particle Stoner excitations and collective spin-wave excitations. Therefore both the energies and life times of the excitations can be addressed.

The presentation will start with the discussion of the magnetic excitations in bulk Heusler alloys. Next, different aspects of the spin dynamics of thin films will be considered.

By the example of the Heusler alloys we will show that the number of the spin-wave modes correlates with the number of well-defined atomic moments in the unit cell. The difference to the adiabatic theories will be demonstrated. The relation between spin-wave life time and half-metallicity will be discussed.

Turning to the thin films we will show that reduced dimensionality rises new questions concerning the character and life time of the collective excitations. In particular, the formation of the standing waves and the influence of the nonmagnetic substrate on the life time of the spin waves will be addressed. On this basis we will consider the magnetization dynamics driven by the magnetic field applied to a part of the film. The study of such processes is crucial for the design of the nano-scale devices based on the inter-device communication by means of spin waves.

SPIN EXCITATIONS IN ITINERANT FERROMAGNETS

FROM FIRST PRINCIPLES

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The long-range order of the electron spins in magnetic solids gives rise to characteristic excitation modes that preserve the particle number but change the total spin of the electron system. Stoner excitations correspond to single-particle spin-flip transitions whose energies are determined by the exchange splitting between the majority and minority channels. In addition, spin waves appear as low-energy collective excitations that govern the thermodynamic properties at low temperature. Here we explore different approaches to calculate the material-specific spin excitations from first principles. The key quantity is the dynamic transverse spin susceptibility, whose spectral function can be directly related to experimental measurements. Dynamic exchange-correlation effects are treated within time-dependent density-functional theory or many-body perturbation theory. In the latter case, maximally localized Wannier orbitals are used to efficiently obtain the electron-hole vertex of the multiple-scattering matrix, which is constructed with full frequency and wave-vector dependence [1]. Our implementation uses the full-potential linearized augmented-plane-wave (FLAPW) method [2]. For the ferromagnetic transition metals Fe, Co and Ni our results are in good agreement with experimental data and reproduce all important features of the measured spin-wave spectra.

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[2] C. Friedrich, S. Blügel and A. Schindlmayr, *Phys. Rev. B* **81**, 125102 (2010).

Hybrid Functionals within the All-Electron FLAPW Method: Implementation and Applications

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Density-functional theory is exceptionally successful in describing the properties of molecules and solids. However, the commonly used approximations for the exchange-correlation functional - the local-density (LDA) and generalized gradient approximation (GGA) - fail to describe the band gaps and structural properties of a number of semiconducting and insulating materials. The self-interaction error in LDA and GGA is mainly responsible for this shortcoming. It is partly corrected in hybrid functionals, which contain a certain fraction of nonlocal Hartree-Fock exchange. So far, most implementations for periodic systems approximate the presence of the core by pseudopotentials and employ a plane-wave basis set. In this contribution, we present an efficient implementation of the PBE0 and HSE06 functionals within the all-electron full-potential linearized augmented plane-wave method realized in the FLEUR (www.flapw.de) code. We demonstrate the improvement over LDA and GGA for oxide materials and focus in particular on systems where the results obtained with the standard functionals disagree with experimental results.

Locally magnetic nanostructures: interplay between magnetism and electron transport

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Nanosystems consisting of a small magnetic structure bridging two nonmagnetic leads are presently of considerable interest because of a variety of intriguing phenomena such as spin filtering, anisotropic magnetoresistance, low temperature Kondo physics and so on. The magnetic bridge may be just a transition metal atom, or a magnetic molecule, or may even consist of the same metal as the leads, turning spontaneously magnetic, as predicted for Pd or Pt atomic chains [1]. We first discuss the case of Pt nanowire contacts, where recent density-functional theory (DFT) studies predicted a large magnetic moment localized on atomic chain connecting two nonmagnetic leads [2,3]. Strong spin-orbit coupling (SOC) results in large magnetic anisotropy with an easy axis parallel to the chain. Next, we look at the case of light magnetic impurities (Ni, Co, or Fe atoms) adsorbed on a Au nanowire or on a carbon nanotube. Due to very weak SOC (and therefore negligible magnetic anisotropy), the Kondo effects will now play an important role and will modify substantially the DFT conductance at low temperatures. We study these phenomena combining our DFT approach with the subsequent Numerical Renormalization Group solution of appropriate Anderson models [4].

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[4] P. Lucignano et al., Nature Materials 8, 563 (2009); P. Baruselli et al., in preparation.

A first-principles study of the resistivity, Gilbert damping and spin-flip diffusion in $\text{Ni}_{1-x}\text{Fe}_x$ substitutional alloys

COMPUTATIONAL MAGNETISM AT JUELICH 2010

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Using a formulation of first-principles scattering theory that includes disorder and spin-orbit coupling on an equal footing, we calculate the resistivity ρ , spin flip diffusion length l_{sf} and the Gilbert damping parameter α for $\text{Ni}_{1-x}\text{Fe}_x$ substitutional alloys as a function of x . For the technologically important $\text{Ni}_{80}\text{Fe}_{20}$ alloy, permalloy, we calculate values of $\rho = 3.7 \pm 0.05 \mu\Omega \cdot \text{cm}$, $l_{sf} = 5.2 \pm 0.2 \text{ nm}$ and $\alpha = 0.0047 \pm 0.002$ compared to experimental low-temperature values in the range $4.4 - 5.1 \mu\Omega \cdot \text{cm}$ for ρ , $5.0 - 6.0 \text{ nm}$ for l_{sf} and $0.005 - 0.008$ for α indicating that the theoretical formalism captures the most important contributions to these parameters taking into account only elastic scattering.

Proper treatment of the macroscopic variables in multiferroic systems

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Multiferroic materials are a class of insulators which are simultaneously ferroelectric, ferromagnetic and ferroelastic. For a rigorous treatment of their response to external perturbations, it is crucial to establish an internally consistent formulation of the macroscopic degrees of freedom (polarization, magnetization and strain), together with the respective generalized fields (electric field, magnetic field and stress). This is especially true when working at non-trivial electrical or mechanical boundary conditions (i.e. with applied DC bias and/or external pressure), where many of the usual definitions of the response coefficients (e.g. piezoelectric, dielectric or elastic) lead to ambiguities or inconsistencies. To address these issues, I will present a formulation of electrostatics in periodic insulators that is based on scalar quantities (charges and potentials), rather than vector quantities (polarization and electric fields) [1]. I will elucidate these ideas by presenting first-principles results on the non-linear piezoelectric coefficient of PbTiO_3 in high fields. I will also discuss extensions of these strategies to the structural and magnetic degrees of freedom, which are currently under way.

[1] M. Stengel, N. A. Spaldin and D. Vanderbilt, *Nature Physics* **5**, 304-308 (2009).

CALCULATION OF SPIN-ORBIT INDUCED RELAXATION IN TRANSITION METAL FERROMAGNETS

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In transition metal ferromagnets, dissipation of energy and angular momentum from the magnetization proceeds via spin-orbit coupling. A time-dependent magnetization, when combined with spin-orbit coupling, generates electron hole pairs, which relax to the lattice. In pure transition metals, the spin-orbit coupling is intrinsic to the band structure, while for rare earth impurities, it is associated with the defects. The relaxation of the electron hole pairs can be through phonons, defects, or alloy scattering. Calculations of the Gilbert damping parameter based on this model and the local spin density approximation agree quantitatively with measurements for Fe, Co, and Ni. The presence of an electrical current modifies the distribution of electrons near the Fermi surface to reflect the net flow of electrons. The modified distribution changes the Gilbert damping and the change in the Gilbert damping gives the non-adiabatic spin-transfer torque parameter, which plays a crucial role in current induced domain wall motion.

RELATIVISTIC CORRECTIONS TO SPIN-INTERACTIONS IN NANOSCALE MAGNETS

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The use of traditional Heisenberg spin-models including on-site magnetic anisotropies and magnetic dipole-dipole interactions has proved insufficient in case of magnetic objects on the nanoscale. Beside the inter-site magnetic anisotropies that have crucial importance even for the finite temperature magnetism of bulk magnets, the role of the Dzyaloshinskii-Moriya (DM) interaction gets largely enhanced in reduced dimension. Well-known examples are the magnetic pattern formation [1] and the homochirality of domain walls [2] in ultrathin films.

Multiple scattering theory provides a straightforward tool to calculate spin-interactions in metals within the framework of relativistic electron theory. I briefly discuss two different methods to accomplish this task. Related to the relativistic torque method, I mainly focus on the calculation of spin-wave spectra [3] by showing that the chiral degeneracy of the magnon spectrum can be lifted due to the presence of DM interactions [4]. I discuss the symmetry conditions under which such a chiral asymmetry occurs. Calculations for an Fe monolayer on W(110) will be presented, with particular emphasis on the possibility to directly measure the DM interactions in ultrathin films.

A new strategy to calculate spin-interactions based on the relativistic Disordered Local Moment picture [5] will also be introduced. Application of the method to Mn/W(001) is clearly consistent with the spin-spiral formation reported recently in the literature. [6] Moreover, I shall highlight the possibility for a direct evaluation of higher order spin-interactions within this method.

[1] M. Bode *et al.*, Nature **447**, 190 (2007)

[2] M. Heide *et al.*, Phys. Rev. B **78**, 140403(R) (2008)

[3] L. Udvardi *et al.*, Phys. Rev. B **78**, 140403(R) (2003)

[4] L. Udvardi and L. Szunyogh, Phys. Rev. Lett. **102**, 207204 (2009)

[5] J.B. Staunton *et al.*, Phys. Rev. B **74**, 144411 (2006)

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ANISOTROPIC MAGNETORESISTANCE AND ANOMALOUS HALL EFFECT IN RANDOM FERROMAGNETIC ALLOYS

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The talk reviews recent progress in ab initio theory of transport properties of spin-polarized metallic systems in presence of spin-orbit interaction. Our approach is based on evaluation of the full conductivity tensor within the Kubo linear response theory with impurity scattering due to chemical randomness. The alloy disorder is taken into account by means of the coherent-potential approximation (CPA) implemented in the tight-binding linear muffin-tin orbital (TB-LMTO) method. The spin-orbit interaction is treated as an on-site perturbation to the scalar-relativistic TB-LMTO Hamiltonian, the velocity operators are reduced to intersite hopping elements, and the CPA-vertex corrections to the conductivity tensor are included.

The developed theory is applied to cubic binary transition-metal alloys FeCo (bcc), NiCo (fcc), NiFe (fcc) and NiMn (fcc) for which selected concentration trends are discussed: (i) a strong deviation of the isotropic resistivity from the Nordheim rule in FeCo alloys, (ii) a big anisotropic magnetoresistance in NiCo and NiFe alloys, and (iii) the change of sign of the anomalous Hall effect. Particular attention is paid to the dilute limit (bcc Fe, fcc Ni), where the Kubo theory provides an alternative description of the anomalous Hall conductivity of non-random magnets formulated recently in terms of their band structure and the Berry curvature.

NON-ADIABATIC SPIN TORQUE IN MAGNETIC DOMAIN WALLS FROM FIRST-PRINCIPLES

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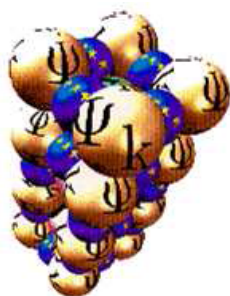
The manipulation of magnetic domains using spin-polarized currents has been proposed as an efficient way of storing and processing information. Controlling current-driven domain wall (DW) motion is, however, non-trivial in practice. The DW velocity is proportional to the ratio between the effective out-of-plane spin-transfer torque parameter β and the Gilbert damping coefficient α but little is known about the numerical value of β and how it depends on material composition, structure etc. In a study of (Ga,Mn)As based upon an empirical four-band Hamiltonian, β was found to be two orders of magnitude larger than α and the energy dissipation resulted mainly from a combination of strong DW scattering and intrinsic spin-orbit interaction.¹

In the present work, we calculate the full scattering matrix for magnetic DWs from first-principles² including spin-orbit coupling using a TB-MTO basis and use it to evaluate the damping parameters α and β for DWs in clean Fe, Co, and Ni. We discuss how the ratio between β and α depends on the material studied and on the width and type of the DW and also how the same approach can be applied to study damping in alloys where the impurity scattering becomes important. Our results can provide valuable guidance for experimental investigations.

¹K. M. D. Hals, A. K. Nguyen, and A. Brataas, *Phys. Rev. Lett.* **102**, 256601 (2009).

²K. Xia, M. Zwierzycki, M. Talanana, P. J. Kelly, and G. E. W. Bauer, *Phys. Rev. B* **73**, 064420 (2006).

Psi-k Network : Towards Atomistic Materials Design



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PSI-K WORKSHOP FINANCE REPORT

Title of the Workshop	Computational Magnetism and Spintronics 2010
Workshop Organisers	Stefan Blügel, Yuriy Mokrousov and Alexander Shick
Location of the Workshop	Bonn, Gustav-Stresemann-Institut, Germany
Dates of the Workshop	May 10 th -12 th 2010
Total Grant from Psi-k	€ 9500

EXPENDITURE

WORKSHOP DELEGATES / SPEAKERS			
Name and Country of Claimant	Travel	Accommodation	Total (€'s)
Patrick Rinke, Germany	70,20	187,00	257,20
Alexander Smogunov, France	196,00	261,00	457,00
Silvia Picozzi, Italy	403,22	164,95	568,17
Ilja Turek, Czech Republic	296,80	251,00	547,80
Hubert Ebert, Germany	119,40	174,00	293,40
Leonid Sandratskii, Germany	190,00	251,00	441,00
Massimiliano Stengel, Spain	356,00	251,00	607,00
Claude Ederer, Ireland	331,15	251,00	582,15
Arthur Ernst, Germany	39,25	87,60	126,85
Rossitza Pentcheva, Germany	269,61	174,00	443,61
Uwe Gerstmann, Germany	57,50	267,00	324,50
Arno Schindlmayr, Germany	50,00	164,00	214,00
Antonio Costa, USA	843,64	251,00	1094,64
Alexander Shick, Czech Republic	0,00	174,00	174,00
Sergii Khmelevskiy, Austria	158,00	251,00	409,00
Roberto Muniz, Brazil	762,95	251,00	1013,95
Total Travel & Accommodation			€ 7554,27

WORKSHOP REFRESHMENTS / CONFERENCE DINNERS			
Date	Tea / Coffee	Lunch / Dinner	Total (€'s)
May 10 th 2010	940,72	125,6	1066,32
May 11 th 2010	940,72	125,6	1066,32
May 12 th 2010	470,36	125,6	595,96
Total Refreshments			€ 2728,6

MISCELLANEOUS EXPENDITURE		
Details	Total (€'s)	
Projector	390,00	
Poster stands	94,00	
Additional accommodation	1629,75	
Conference dinner	890,00	
Total Miscellaneous		€ 3003,75

Total Travel & Accommodation	€ 7554,27
Total Refreshments	€ 2728,6
Total Miscellaneous	€ 3003,75

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