MA 51: Electron Theory of Magnetism

Time: Friday 9:30–12:00 Location: HSZ 401

MA 51.1 Fri 9:30 HSZ 401

A coherent relativistic description of spin and orbital magnetisation of solids — •Hubert Ebert and Sergiy Mankovsky — Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland

Recently, a definition for the orbital magnetisation of magnetic solids was suggested using a Bloch representation of the electronic structure [1]. Results for the spin-orbit induced magnetisation of Fe, Co and Ni based on this approach were presented by various authors [2]. To avoid the approximations and limitations of these investigations we present a coherent relativistic definition for the total magnetisation that is derived from the interaction of the total electronic current density with an external magnetic vector potential. Representing the electronic structure in terms of the Green function using the KKR band structure method leads to two terms that can be related to the Van Vleck and Landau contributions of the magnetic susceptibility [3]. A decomposition of the total magnetisation may be obtained by subtracting the spin part, that can be unambiguously determined, from the total magnetisation. Another route is to make use of the Gordon decomposition of the total electronic current density leading in a natural way to a spin and orbital contribution. Numerical results for the elemental ferromagnets Fe, Co and Ni will be presented and discussed.

[1] J. Shi et al., PRL **99**, 197202 (2007)
[2] D. Ceresoli et al. PRB **81** 060409(R) (2010);
M. G. Lopez et al., PRB **85** 014435 (2012)
[3] S. Mankovsky and H. Ebert, PRB **74**, 054414 (2006)

MA 51.2 Fri 9:45 HSZ 401

Exchange interactions and Curie temperature of MnSi: A density functional study — •Giovanna Lani, Phivos Mavropoulos, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present a theoretical investigation of zero and finite temperature properties of bulk MnSi in the B20 structure. MnSi is known to pose a theoretical challenge, as its magnetic moment is overestimated by a factor two within the LDA and GGA approximations to DFT. Therefore, employing two different all-electron approaches, namely the FLAPW and KKR methods, we investigate how constraining the magnetic moment to the experimental value affects the electronic structure of MnSi. By mapping the results of DFT calculations onto a Heisenberg Hamiltonian, we extract the exchange parameters. We find that they exhibit long-range oscillations and we argue that while some of their features are independent of the value of the magnetic moment, others are not and this can be attributed to changes in the Fermi surface topology as a function of the moment. The Curie temperature, estimated via a Monte Carlo method, agrees with the available measurements only when the moment is constrained to the experimental value. This finding is further validated by including longitudinal moment fluctuations within a static mean field theory with a KKR-CPA disordered local moment calculation in the spirit of the Hubbard III approximation.

MA 51.3 Fri 10:00 HSZ 401

Ab-initio spin dynamics for clusters — •Laszlo Udvardi, Levente Rozsa, and Laszlo Szunyogh — Dept. of Theor. Phys., TU Budapest, Hungary

Ab initio atomistic spin dynamics simulations provide a way to theoretically investigate systems containing from a few dozen to a few thousand atoms. These methods are based on the numerical solution of the stochastic Landau-Lifshitz-Gilbert (LLG) equation. In most of the cases the torque driving the motion of the spins is determined by means of a Heisenberg model with ab-inito parameters.

In the present work we propose a method where the torque is calculated directly from the density functional theory without the need of underlying Heisenberg model. The electronic structure of the cluster is determined by applying the embedded cluster method using the relativistic Korringa-Kohn-Rostoker method. The torque rotating the spins in the cluster is calculated within the framework of the magnetic force theorem as the derivatives of the band energy with respect of the transverse change of the magnetization.

The method is applied for a 10 atoms long linear Co chain on Au (001) surface. The magnetic ground state is turned out to be a spin spiral due to the Dzyaloshinsky-Moriya interaction. The results of the simulations are in good agreement with the results of the analytically solvable Heisenberg chain with nearest neighbor exchange coupling. The behaviour of the switching between the two degenerate ground states was also studied by means of both ab-initio and model calculations.

MA 51.4 Fri 10:15 HSZ 401

The phase diagram of the xxz model on the triangular lattice — •Daniel Sellmann, XUE-FENG ZHANG, and Sebastian Eggert — University of Kaiserslautern, Germany

The Heisenberg model on the triangular lattice was proposed as the first example of a spin-liquid by Anderson in the early 70s. Even though the isotropic Heisenberg model is by now well understood and known *not* to be a spin-liquid in the modern sense, there are still no quantum many-body simulations which have explored the full phase diagram of the xxz model on the triangular lattice. We now present DMRG calculations on order parameters and entanglement measures in order to establish the quantitative phase diagram as a function of field and Ising anisotropy. The transition to the xy-phase is always first order, but there is a novel tricritical point at the transition to the 1/3-Neel phase. The neel phase is connected to two different supersolid-type phases by second order phase transitions, one of which curiously turn first oder in the Ising limit.

MA 51.5 Fri 10:30 HSZ 401

Ab initio calculation of crystal field parameters for single Holmium atoms at a surface — •Martin Hoffmann[1,2], Matthias Geilhufe[2], Sergey Ostanin[2], Wolfram Hergert[1], Ingrid Mertig[1,2], and Arthur Ernst[2,3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [3]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany

The direction of the magnetic moments of atoms at a surface depends strongly on the anisotropy of the underlying material. In most cases, the determination of the simple uniaxial anisotropy is sufficient to describe the orientation of the moments. However, this is only the first term in the more general crystal field Hamiltonian $\mathcal{H}$. Higher terms couple e.g. different sublevels of the energy spectrum of an adsorbed atom.

Based on the electronic density of the substrate and the ad-atom, the parameters for this $\mathcal{H}$ can be calculated by ab-initio methods. We will present the implementation of this scheme for the Korringa-Kohn-Rostoker Green's function method.

As application example, we calculated for a single Holmium (Ho) atom at a Pt(111) surface at first the position and the electronic and magnetic properties. With theses quantities we obtained the crystal field parameters for $\mathcal{H}$, which can be further solved by exact diagonalization for the magnetic states of Ho. The resulting energy splitting is in very good agreement with experimental results.

MA 51.6 Fri 10:45 HSZ 401

Crystal field and magnetism with Wannier functions: rare earth ions in oxides — •Pavel Novak — Institute of Physics ASCR, Cukrovarnicka 10, 162 00 Praha 6, Czech Republic

During the last two years we developed a scheme, which was successfully used to determine the crystal field parameters of trivalent rare earth ions in oxides. These parameters were then inserted in atomic-like program which, besides the crystal field, takes into account the 4f-4f electron repulsion, spin-orbit and Zeeman interactions. The agreement of the calculated and experimental splitting of rare earth multiplets was very good (within meV) and also magnetism of the RE multiplets was correctly described. The method was already applied to more than fifty systems: rare earth containing aluminates, galates, cobaltites and manganites with orthorhombic perovskite structure, yttrium aluminium and lutetium aluminium garnets containing rare earth impurities and rare earth layered hexagonal cobaltates. In the present contribution the method is reviewed and applied to selected rare earth compounds. Accuracy and limits of the method is also discussed.

P. Novak, K. Knizek and J. Kunes, Phys. Rev. B 87, 205139 (2013).

P. Novak, K. Knizek, M. Marysko, Z. Jirak and J. Kunes, J. Phys.: Condens. Matter 25, 446001 (2013).

MA 51.7 Fri 11:00 HSZ 401

Electronic structure and magnetic properties of Cr-Sb compounds with NiAs structure — •Sergiy Mankovsky[1], Gerhard Kuhn[1], Svitlana Polesya[1], Matthias Regus[2], Wolfgang Bensch[2], and Hubert Ebert[1] — [1]Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Max-Eyth-Str. 2, D-24118 Kiel, Deutschland

The electronic structure and magnetic properties of binary Cr-Sb compounds with NiAs crystal structure have been investigated via Density Functional Theory (DFT) band structure calculations using the Korringa-Kohn-Rostoker Green function (KKR-GF) method. The finite temperature magnetic properties were studied by means of Monte Carlo simulations based on the Heisenberg model with the exchange coupling parameters calculated from first principles. The modification of the properties of Cr-Sb compounds due to substitution of Cr by 3*d*-elements is also studied. In particular, the magnetic phase diagram of the $Cr_{1-x}Mn_xSb$ alloy system with NiAs structure was calculated. At low temperatures, it shows stable collinear FM and AFM states for the Mn- and Cr-rich sides, respectively, and a non-collinear magnetic structure in the middle region of concentrations. These findings are fully in line with experimental data.

MA 51.8 Fri 11:15 HSZ 401

Electronic structure and magnetic anisotropy of $Sm_2Fe_{17}N_x$ — •Masako Ogura[1,2] and Hisazumi Akai[3] — [1]Ludwig-Maximilians-University Munich, Munich, Germany — [2]Osaka University, Toyonaka, Japan — [3]University of Tokyo, Kashiwa, Japan

Electronic structure and magnetic properties of $Sm_2Fe_{17}N_x$ are studied on the basis of the first-principles electronic structure calculation in the framework of the density functional theory. It is experimentally known that the magnetism of Sm_2Fe_{17} is enhanced when N is added. In the present study, the magnetic properties of the system as a function of the N concentration are discussed. Although the main origin of the enhancement of the magnetism is the volume enhancement due to the addition of N, the hybridization between the Fe 3d states and the N 2p states also plays an important roll. In addition, the electron transfer between Sm and N affects the magnetic anisotropy.

MA 51.9 Fri 11:30 HSZ 401

Fast algorithm for conductance of layered systems — •Vaclav Drchal[1], Josef Kudrnovsky[1], and Ilja Turek[2] — [1]Inst. of Physics, Acad. Sci., Praha, Czech Republic — [2]Inst. of Physics of Materials, Brno, Czech Republic

We developed a highly efficient method to calculate the conductance of disordered multilayer systems that can be represented by lateral supercells with random occupation of lattice sites by atoms. Stacking of supercells in the growth direction is arbitrary. The method employs the surface Green functions and it is of $O(L)$ type, where L is the number of layers. For large L the conductance behaves as $C(L) = \sigma L$, where σ is a longitudinal conductivity. The method is illustrated on disordered magnetic alloys and on a graphene sheet with adsorbed magnetic atoms.

MA 51.10 Fri 11:45 HSZ 401

The Fermi-sea term in relativistic LMTO transport theory for random alloys — •Ilja Turek[1], Josef Kudrnovsky[2], and Vaclav Drchal[2] — [1]Institute of Physics of Materials, Acad. Sci. Czech Rep., Brno, Czech Republic — [2]Institute of Physics, Acad. Sci. Czech Rep., Prague, Czech Republic

We present formulation of the so-called Fermi-sea contribution to the conductivity tensor of spin-polarized random alloys within the fully relativistic tight-binding LMTO method and the coherent potential approximation (CPA). We show that the configuration averaging of this contribution is surprisingly simple, since it leads to the CPA-vertex corrections that are solely due to the energy dependence of the average single-particle propagators. Moreover, we prove that the Fermi-sea term is indispensable for the invariance of the anomalous Hall conductivities with respect to the particular LMTO representation used in numerical implementation. The calculations for ferromagnetic 3*d* metals (Fe, Co, Ni) and their selected random binary alloys will be presented and their results will be compared with the previous study [1] based only on the Fermi-surface contribution. [1] I. Turek et al., Phys. Rev. B 86, 014405 (2012).