MA 25: Electron Theory of Magnetism

Time: Wednesday 9:30–10:45 Location: H 0112

MA 25.1 Wed 9:30 H 0112

Magnetic Compton profiles of Fe and Ni corrected by dynamical electron correlations — •Diana Benea[1], Jan Minar[2], Serghey Mankovsky[2], Liviu Chioncel[3,4], and Hubert Ebert[2] — [1]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania — [2]Chemistry Department, University of Munich, Germany — [3]Augsburg Center for Innovative Technologies, University of Augsburg, Germany — [4]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

Magnetic Compton profiles (MCPs) of Ni and Fe have been calculated using a combined Density Functional and many-body theory approach. At the level of the local spin density approximation the theoretical MCPs does not describe correctly the experimental results around the zero momentum transfer. In this work we demonstrate that inclusion of electronic correlations as captured by Dynamical Mean Field Theory (DMFT) improves significantly the agreement between the theoretical and the experimental MCPs. In particular, an energy decomposition of Ni MCPs gives indication of spin polarization and intrinsic nature of Ni 6 eV satellite, a genuine many-body feature.

MA 25.2 Wed 9:45 H 0112

Magnetic anisotropy energy of disordered and ordered tetragonal FeCo alloys — •Ilja Turek[1,3], Josef Kudrnovsky[2], and Karel Carva[3] — [1]Institute of Physics of Materials ASCR, Brno, Czech Republic — [2]Institute of Physics ASCR, Prague, Czech Republic — [3]Dept. of Condensed Matter Physics, Charles Univ., Prague, Czech Republic

We present results of *ab initio* calculations of the uniaxial magnetic anisotropy energy (MAE) in disordered body-centered tetragonal (bct) FeCo alloys as well as in alloys with a partial $L1_0$ order. The latter systems are simulated by a two-sublattice model with different sublattice compositions. The calculations employ the relativistic TB-LMTO method and the coherent potential approximation (CPA) which enables us to scan the entire intervals of both concentration variables and a broad range of the bct c/a-ratio. For the homogeneous alloys, we have found that the huge maximum MAE of about 800 μeV/atom, obtained previously in a simple virtual crystal approximation, overestimates the MAE of the random alloys in the CPA at least by a factor of four. This effect is due to the strong disorder-induced scattering in the minority spin channel, manifested by a strong broadening of the Bloch spectral functions near the Fermi energy. For the ordered alloys, we have found that the maximum $L1_0$ order compatible with a given Co concentration can bring the MAE up to high values around 500 μeV/atom. However, these high MAEs are significantly reduced by small perturbations of the perfect atomic order. Relation of the MAEs to the orbital magnetic moments will also be presented and discussed.

MA 25.3 Wed 10:00 H 0112

Magnetism without d Electrons from First Principles: Ground State and Spin Dynamics of the Diamond (111) Surface — •Guntram Fischer[1], Pawel Buczek[2], Wolfram Hergert[1], Evgeny Chulkov[3], Victor Tugushev[3], Leonid Sandratskii[2], and Arthur Ernst[2] — [1]University of Halle, Halle, Germany — [2]University of San Sebastian, San Sebastian, Spain — [3]Max Planck Institute for Microstructure Physics, Halle, Germany

The polar (111) surface of diamond has been studied within the framework of density functional theory using a KKR Greens Functions formalism. In agreement with experiment [1], we find an antiferromagnetic ground state driven by a Stoner instability in the manifold of p states. The spin-flip spectrum is determined from time dependent density functional theory [2]. The magnon dispersion is also analyzed in the frozen magnon approach and the Néel temperature is estimated using Monte Carlo simulations [3].

[1] Ramaker *et al.*, Solid State Comm. **63**, 335 (1987)
[2] Buczek *et al.*, PRL **102**, 247206 (2009)
[3] Fischer *et al.*, PRB **80**, 014408 (2009)

MA 25.4 Wed 10:15 H 0112

Electronic structure of ferromagnetic Heusler compounds from meta-GGA density functionals — •Markus Meinert, Jan Schmalhorst, and Günter Reiss — Dünne Schichten und Physik der Nanostrukturen, Fakultät für Physik, Universität Bielefeld, 33501 Bielefeld

Modern meta-GGA density functionals have recently been implemented self-consistently within the GPAW code [1]. We apply the non-empirical revTPSS [2] and the highly parametrized M06-L [3] functionals to the electronic structure problem of ferromagnetic Heusler compounds and other test cases. Changes in the description of the ferromagnetic or half-metallic ground states with respect to LSDA or PBE results will be discussed. [1] J. Enkovaara et al., J. Phys.: Condens. Matter 22, 253202 (2010) [2] J. P. Perdew et al., PRL 103, 026403 (2009) [3] Y. Zhao and D. G. Truhlar, J. Chem. Phys. 125, 194101 (2006)

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