MA 20: Electron Theory of Magnetism

Time: Tuesday 11:00–12:45 Location: HSZ 103

MA 20.1 Tue 11:00 HSZ 103

Sensitivity of the calculated magnetocrystalline anisotropy of ad-atoms on the treatment of the substrate — •Ondrej Sipr[1], Sven Bornemann[2], Jan Minar[2], and Hubert Ebert[2] — [1]Institute of Physics of the ASCR v.v.i., Prague, Czech Republic — [2]Universitat Munchen, Department Chemie, Munchen, Germany

The magnetocrystalline anisotropy energy (MAE) of Fe and Co adatoms, monolayers and surface superstructures on the highly polarizable Pt(111) surface is investigated. It turns out that the finite thickness of the slab which is conventionally used to represent the substrate and interaction between the ad-atoms in neighboring surface supercells affect calculated values of the MAE much more profoundly than they affect calculated values of magnetic moments. Reliable theoretical values for the MAE thus cannot be obtained if the substrate is represented by a slab of less than 7-10 atomic layers or if the surface supercell describing the ad-atoms is so small that the relative site occupation by the ad-atoms is more than few percents.

MA 20.2 Tue 11:15 HSZ 103

Magnetic interactions of iron — •Frank Dietermann and Manfred Fähnle — Max-Planck Institut für Metallforschung, Stuttgart

We investigate the adiabatic magnetic energy landscape of iron in the bcc and fcc crystal structure by constrained spin density functional theory. We use this data, to fit the interaction coefficients of an extended Heisenberg model and of a Spin-Cluster-Expansion [1] and compare the two models. We also discuss the influence of the type of reference configurations considered - e.g. spin spirals with constant opening angle, spin spirals with various opening angles or supercells.

[1]R.Drautz and M.Fähnle, Phys.Rev. B **69**, 103303 (2004)

MA 20.3 Tue 11:30 HSZ 103

Ab-initio calculation of the Gilbert damping parameter for transition metal alloys — •Sergiy Mankovsky, Diemo Ködderitzsch, and Hubert Ebert — Dept. Chemie/Phys. Chemie, Universität München, Butenandtstr. 11, D-81377 München, Deutschland

We present a theoretical approach for the calculation of the Gilbert damping parameter α using the linear response formalism as implemented within the KKR Green's function technique. The expression for the Gilbert damping parameter was obtained in the adiabatic approximation following the ideas of Brataas et al.[1] This approach was applied to various metal alloy systems. The results for the Gilbert damping parameters are compared with corresponding theoretical results obtained recently by Starikov et al. [2] as well as available experimental data. The theoretical results agree very well among each other demonstrating the equivalence of the two different approaches used. The experimental values for α are reproduced quite well by the calculations concerning the concentration dependence, but are in general larger. This is ascribed to the influence of thermal fluctuations ignored so far in the calculations.

[1] A. Brataas, Y. Tserkovnyak, and G. E. W. Bauer, Phys. Rev. Lett. **101**, 037207 (2008).

[2] A. A. Starikov, P. J. Kelly, A. Brataas, Y. Tserkovnyak and G. E. W. Bauer, accepted to Phys. Rev. Lett. (2010)

MA 20.4 Tue 11:45 HSZ 103

Order and phase stability in CoPt: the role of magnetism. — •Sondes Karoui[1], Hakim Amara[1], Francois Ducastelle[1], and Bernard Legrand[2] — [1]LEM, ONERA-CNRS, BP72 92322 Châtillon Cedex, France — [2]SRMP, CEA, Saclay, France

Transition metal nano-alloys (FePd, CoRh, and CoPt) are innovative new materials whose size and chemical composition govern their physical and chemical properties. CoPt, the focus point of this study, had been duly studied in the bulk phase both experimentally and theoretically. There exists a large array of results that clearly hint at the importance of magnetism, and the stabilization that it brings to the system. Indeed, we strongly believe that the crystallographic order present in CoPt can be attributed to the alloy's inherent magnetic character.

To point out this effect, Density Functional Theory calculations have been performed using the ABINIT code with and without magnetism. We report on the influence of spin polarized calculations on structure stabilization in bulk Co and Pt as well as the alloy's various crystallographic phases: ordered L1o, L12, and disordered FCC. This approach corresponds to a quantitative first step towards better understanding the role of magnetism at the atomic scale.

Reference 1 (submitted): S. Karoui, H. Amara, F. Ducastelle, and B. Legrand, First principle study of order and magnetism in Co(1-x)Pt(x).

MA 20.5 Tue 12:00 HSZ 103

Magnetic properties of strongly correlated transition metal oxides studied using LSDA+U — •Gerhard Kuhn[1], Jan Minár[1], Diemo Ködderitzsch[1], Igor di Marco[2], Sergiy Mankovskyy[1], and Hubert Ebert[1] — [1]Universität München Department Chemie, Physikalische Chemie, Haus E2.033, Butenandtstr. 5-13, D-81377 München — [2]Ångströmlaboratoriet, Lägerhyddsvägen 1, 751 20 UPPSALA, SWEDEN

The magnetic properties of strongly correlated systems (MnO, FeO, CoO, NiO) in different magnetic structures (anti ferromagnetic (AF) 1, anti ferromagnetic (AF) 2, ferromagnetic (FM)) were investigated by the LSDA+U formalism implemented within the Korringa-Kohn-Rostoker (KKR) Green's function method. Calculations were performed fully relativistically as well as scalar relativistically using both, the atomic sphere approximation and a full potential formalism. Spin and orbital magnetic moments were calculated. The exchange coupling constants have been determined by a mapping of energy differences of different magnetic structures onto a Heisenberg-model. Further, the exchange coupling constants have been calculated by a relativistic generalization of Lichtenstein's formula.

MA 20.6 Tue 12:15 HSZ 103

Ab-initio description of the magnetic shape anisotropy due to the Breit interaction — •Sven Bornemann, Jan Minar, Jürgen Braun, Diemo Ködderitzsch, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München, 81377 München

A quantum-mechanical description of the magnetic shape anisotropy, that is usually ascribed to the classical magnetic dipole-dipole interaction, has been developed. This is achieved by including the Breit-interaction, that can be seen as an electronic current-current interaction in addition to the conventional Coulomb interaction, within fully relativistic band structure calculations. The major sources of the magnetic anisotropy, spin-orbit coupling and the Breit-interaction, are treated coherently this way. This seems to be especially important for layered systems for which often both sources contribute with opposite sign to the magnetic anisotropy energy. Applications to layered transition metal systems are presented to demonstrate the implications of this new approach in treating the magnetic shape anisotropy.

MA 20.7 Tue 12:30 HSZ 103

Ground state properties that can be derived from total energy calculations — •Liviu Chioncel — Augsburg Center for Innovative Technologies, University of Augsburg, Germany

The temperature dependence of elastic constants for simple transition metal elements has been calculated using a combined first-principles and many-body theory. The thermal expansion has a normal linearly decreasing contribution to the elastic constant, while the electronic contribution is determined by the unique character of Coulomb correlations and may lead to anomalous temperature effects.