MA 5: Electron Theory of Magnetism

Time: Monday 11:00–13:15 Location: HSZ 103

MA 5.1 Mon 11:00 HSZ 103

Ab initio **calculation of the full anti-symmetric conductivity tensor for magnetically ordered systems** — •Stephan Lowitzer, Diemo Ködderitzsch, and Hubert Ebert — Department Chemie und Biochemie, LMU München, Butenandtstraße 11, 81377 München

The *ab initio* calculation of the full anti-symmetric conductivity tensor for magnetically ordered systems is up to now a very difficult task. We present the first results of a recent investigation on the transition metal alloys $Fe_{1-x}Ni_x$ and $Co_{1-x}Pd_x$. For these we employed the fully relativistic Korringa-Kohn-Rostoker (KKR) band structure method in conjunction with the coherent potential approximation (CPA) alloy theory. The calculation of the conductivity tensor is based on the expressions by Středa and its extension by Crépieux and Bruno, that contain the Kubo-Greenwood expression for the symmetric conductivity tensor as a special case.

MA 5.2 Mon 11:15 HSZ 103

Spin-polarized relativistic optimized effective potential method for open-shell atoms and magnetic solids — •Diemo Ködderitzsch[1], Hubert Ebert[1], and Eberhard Engel[2] — [1]Ludwig-Maximilians-Universität, D-81377 München, Germany — [2]J. W. Goethe-Universität, D-60438 Frankfurt, Germany

We introduce the concept of the exact orbital-dependent exchange into relativistic **spin**-density functional theory and give a relativistic formulation of the optimized effective potential method (ROEP). [1,2]

We first present its application to open-shell atoms and discuss the relative importance of exchange splitting and spin-orbit coupling as well as the relative stability of $3d^{n-1}4s^2$ and $3d^n4s^1$ configurations in case of $3d$ transition-metal elements.

In addition, we present an extension of the formalism to solids and its implementation within the KKR formalism.[3] The scheme is an all electron approach treating core and band states formally on the same footing. We use exact exchange (EXX) as approximation to the xc-functional which for the valence states is reformulated in terms of the electronic Green's function. Numerical four-component wave functions for the description of the ingredients of the ROEP integral equation are employed. We present and discuss the application of the formalism to non-magnetic alkali metals and to magnetic $3d$ transition-metals.

[1] D. Ködderitzsch, H. Ebert, E. Engel, PR**B 77**, 045101 (2008)
[2] E. Engel, D. Ködderitzsch, H. Ebert, PR**B 78**, accepted (2008)
[3] D. Ködderitzsch, H. Ebert, H. Akai, E. Engel, J. Phys: Condens. Matter, accepted (2008)

MA 5.3 Mon 11:30 HSZ 103

Investigating magnetic properties of Heusler compounds with *ab initio* **calculations** — •Jan Thoene[1], Gerhard H. Fecher[1], Stanislav Chadov[1], Claudia Felser[1], and Jürgen Kübler[2] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Institut für Festkörperphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

We have studied the magnetic properties of various Heusler compounds with Density Functional Theory calculations. The Kohn-Sham equations were solved using the Korringa-Kohn-Rostoker Green function formalism. Heisenberg exchange energies have been calculated employing the local force theorem to derive total energy changes associated with a rotation of the local magnetisation direction. The exchange constants were used to evaluate finite-temperature magnetic properties as Curie temperatures and spin-stiffness. Further, the influence of local correlation effects on the magnetic properties was investigated in terms of the Dynamical Mean-Field Theory.

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MA 5.4 Mon 11:45 HSZ 103

Local correlation effects in $Co_2Mn_{1-x}Fe_xSi$ Heusler alloys — •Stanislav Chadov[1], Gerhard H. Fecher[1], Claudia Felser[1], Jan Minár[2], Jürgen Braun[2], and Hubert Ebert[2] — [1]Johannes Gutenberg University Mainz, Germany — [2]Ludwig Maximillians University Munich, Germany

Strongly correlated electron systems possess an important entry among the Heusler materials. Of the special technological interest are $Co_2Mn_{1-x}Fe_xSi$ alloys which being highly spin-polarized systems exhibit the highest known magnetic moments ranging from 5 to 6 μ_B and the Curie temperatures from 985 to 1100 K. Former theoretical studies evidence the local correlation as an important mechanism responsible for their extreme magnetic properties. We analyze this mechanism by studying the electronic structure with *ab-initio* calculations combining the well-known LSDA approach and the state of the art many-body DMFT scheme. The approach is implemented within the KKR Green's function method. We find both static and dynamic local correlations as an essential ingredient in a description of the electronic structure. Results obtained for the magnetic moments and the photoemission spectra are much improved comparing to the plain LSDA and found to be in a good agreement with experiment. In addition we also discuss the correspondence between the physical properties and the certain types of the many-body interaction.

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MA 5.5 Mon 12:00 HSZ 103

Atom- and bond-resolved analysis of the magnetic anisotropy in multicomponent systems — •Sergej Subkow[1], Matej Komelj[2], and Manfred Fähnle[1] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

For the understanding of the magnetic anisotropy in multicomponent systems like compounds (e.g., FePt) or multilayer systems it would be helpful to subdivide the total anisotropy energy into contributions arising from various atoms or from various bonds between the atoms. The usefulness and the limitation of such type of analysis is assessed critically for four different approaches.

a) procedures based on the magnetic force theorem [1]

b) the relation of Bruno [2]

c) the covalent bond energy [3]

d) the method of switching off the spin-orbit coupling at various atoms [4].

[1] T. Burkert et al., Phys. Rev. B71, 134411 (2005).
[2] C.-G. Duan et al., Appl. Phys. Letters 92, 122905 (2008).
[3] G. Bester and M. Fähnle, Phys. Rev. B72, 212405 (2005).
[4] M. Komelj, D. Steiauf, and M. Fähnle, Phys. Rev. B73, 134428 (2006).

MA 5.6 Mon 12:15 HSZ 103

Lifshitz transitions in FePt due to a canted magnetic field — •Hongbin Zhang and Manuel Richter — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

By density functional calculations, we show that in $L1_0$ FePt, a canted magnetic field can induce changes of the topology of the Fermi surfaces. This is a new driving force for such electronic topological transitions (also called Lifshitz transition) besides pressure, doping, and magnetic field of arbitrary direction. To elucidate its effects, we estimate the variation of thermopower using a simple two-band model. It is shown explicitly, that due to interband scattering, thermopower would have singular behavior at such transitions. However, strong smearing by chemical disorder will make it hard to observe such anomalies experimentally.

MA 5.7 Mon 12:30 HSZ 103

A new scheme to calculate the exchange coupling tensor — •Sergey Mankovsky and Hubert Ebert — Dept. Chemie und Biochemie/Phys. Chemie, Universität München, München, Deutschland

A new scheme to calculate the exchange coupling tensor $\underline{\underline{J}}_{ij}$ describing in a phenomenological way the anisotropic exchange coupling of two moments in a magnetically ordered system is presented. The ab-initio approach is based on spin-polarised relativistic multiple-scattering theory within the framework of spin-density functional theory. The scheme is applied to ferromagnetic CrTe as well as the diluted magnetic semiconductor (DMS) system $Ga_{1-x}Mn_xAs$. In the later case the results show that there is a noticeable anisotropy in the exchange coupling present, although not as pronounced as suggested in recent theoretical investigations.

MA 5.8 Mon 12:45 HSZ 103

Spin-wave excitations from time-dependent density-functional theory — Manfred Niesert[1], Arno Schindlmayr[2], Christoph Friedrich[1], and •Stefan Blügel[1] — [1]Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich — [2]Department Physik, Universität Paderborn, 33098 Paderborn

Spin waves constitute an important class of low-energy excitations in magnetic solids with a characteristic material-specific dispersion and a direct relation to magnetization dynamics. Until now most theoretical studies were based on the Heisenberg model of localized spins or on the frozen-magnon method, but neither is applicable to investigate the dynamics of spin waves in metallic systems with itinerant electrons. As a possible solution, time-dependent density-functional theory gives access to the full frequency-dependent transverse spin susceptibility, from which not only the spin-wave dispersion but also the corresponding excitation lifetimes and other spectral information can be extracted. We have developed a practical scheme to calculate spin-wave spectra from first principles within this framework and present results for the prototype transition metals Iron, Cobalt and Nickel. Our implementation uses the full-potential linearized augmented plane-wave (FLAPW) method, and dynamic exchange-correlation effects are in the first instance described by the adiabatic local-density approximation.

MA 5.9 Mon 13:00 HSZ 103

Electronic structure calculations of uranium compounds — •Carsten Neise, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, P.O.B. 270016, D-01171 Dresden Germany

We performed full-potential density functional theory (DFT) calculations on 5f inter-metallic compounds, which have either tetragonal (FD3M, FM3M, I4/MMM) or hexagonal (P6/MMM) symmetry. We used the local spin density approximation (LSDA) in a full relativistic implementation (http://www.fplo.de) to calculate their magnetic properties. Since it is a known error of LSDA to underestimate the orbital moment, we applied orbital polarisation corrections (OPC) [1,2] to these 5f states.
The magnetocrystalline anisotropy energy (MAE) is connected with orbital moments. Hence OPC affects the MAE. Comparing our results with available experimental data in literature, we find a systematic improvement of orbital moments and MAE with applied OPC. Nevertheless these estimates may be seen as an upper bound.

[1] Eriksson, O. and Brooks, M.S.S. and Johansson, B., Phys. Rev. B. **41** (1990), 7311-7314
[2] Eschrig, H. and Sargolzaei, M. and Koepernik, K. and Richter, M., Europhys. Lett. **72** (2005), 611-617