MA 12 Elektronentheorie

Zeit: Samstag 09:00–10:45 Raum: TU EMH225

MA 12.1 Sa 09:00 TU EMH225

Direct Observation of Orbital Magnetism in Cubic Solids — •H. Wende[1], W.D. Brewer[1], A. Scherz[1], C. Sorg[1], K. Baberschke[1], P. Bencok[2], and S. Frota-Pessôa[3] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem, Germany — [2]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France — [3]Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970 São Paulo, S.P. Brazil

We present X-ray magnetic circular dichroism (XMCD) measurements of the orbital/spin magnetic moment ratios of dilute 3*d*-series impurities (Cr,Mn,Fe,Co) in fcc Au and Cu host matrices [1]. These dilute 3*d* impurities in noble metal hosts represent an intermediate case between the nearly atomic configuration and a bulk 3*d*-metal environment, where the usual description includes strong hybridization and crystal field effects. We show the first direct measurement of considerable orbital moments in cubic symmetry for a localized impurity in a bulk metal host. This confirms previous hyperfine structure measurements. Here, it is shown that the unquenching of orbital magnetism depends on a delicate balance of hybridization effects between the local impurity with the host and the filling of the 3d states of the impurity. The results are accompanied by *ab initio* calculations that support our experimental findings.
Supported by BMBF (05 KS4 KEB 5).
[1] W.D. Brewer *et al.*, Phys. Rev. Lett. **93**, 077205-1 (2004).

MA 12.2 Sa 09:15 TU EMH225

Magnetism in gold nanostructures — •Ingo Opahle, Arti Kashyap, Mahdi Sargolzaei, Klaus Koepernik, Ulrike Nitzsche, Manuel Richter, and Helmut Eschrig — IFW Dresden, P.O.B. 270016, D-01171 Dresden, Germany

As a bulk material, gold does not show any sign of ordered magnetism. Nanostructured materials, on the other hand, have been shown in recent years to have surprising features, sometimes completely different from the bulk phase. In a recent experiment [1] evidence for magnetism in small gold clusters was provided.

In this work, the electronic structure of gold nanostructures (monoatomic gold chain, small clusters) is investigated by means of relativistic density functional theory calculations, with a particular focus on tendencies towards magnetic instabilities. A monoatomic gold chain, for example, becomes magnetic at Au-Au nearest neighbour distances close to those of bulk gold. The calculated magnetic moment reaches up to 0.2 μ_B with a dominating contribution of the orbital moment of 0.12 μ_B.
[1] Y. Yamamoto *et al.*, Phys. Rev. Lett. **93**, 116801 (2004).

MA 12.3 Sa 09:30 TU EMH225

Self-consistent determination of magnon dispersions in the s-d(f) exchange model — •Tilmann Hickel and Wolfgang Nolting — Lehrstuhl Festkörpertheorie, Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

In many materials the ferromagnetic order is assumed to be due to an indirect interaction of localized magnetic moments via itinerant electrons of a conduction band. This mechanism is described in the s-d(f) exchange model (also called Kondo-lattice or double-exchange model). Many-body theoretical approaches to the model often focus on the self-energy of the itinerant subsystem, while treating the local-moment subsystem less accurate. We have developed an projection-operator approach to the s-d(f) exchange model that avoids this inequality of the subsystems. It combines the state-of-the-art knowledge on the density of states with a temperature-dependent determination of magnon dispersions and softening effects. In our evaluation we will focus on the latter. Compared to earlier predictions, the obtained magnetization curves yield a further reduction of the paramter regime where ferromagnetism can be expected.

MA 12.4 Sa 09:45 TU EMH225

Ferromagnetic ordering and halfmetallic state in a shandite: $Co_3Sn_2S_2$ — •Helge Rosner[1], Richard Weihrich[2], Walter Schnelle[1], M. Zabel[3], and Claudia Stueckl[3] — [1]MPI for Chemical Physics of Solids, Dresden — [2]Institut für Anorganische Festkörperchemie, Universität Regensburg — [3]Institut für Anorganische Chemie, Universität Göttingen

The recent rapid development in spintronics challenges the search for new magnetic half metals with high Curie temperatures as well as an improved understanding of the underlying microscopic properties. Here, we present a joint experimental and theoretical study of the recently reinvestigated shandite $Co_3Sn_2S_2$ [1]. From magnetic susceptibility, specific heat and resistivity measurements on powder samples we find a phase transition to a ferromagnetic metallic state at 177 K with a saturation moment of 0.87 μ_B/f.u. Full potential electronic structure calculations within the local spin density approximation result in a halfmetallic ferromagnetic groundstate with a moment of 1 μ_B/f.u. and a tiny gap in the minority spin channel. The calculated structure optimization and structure variations show that the size of the gap is rather sensitive to the lattice geometry. Possibilities to stabilize the halfmetallic ferromagnetic behaviour by various substitutions have been studied theoretically and will be discussed in detail.
[1] R. Weihrich *et. al.* Z. Anorg. Allg. Chem. **630**, 1767, (2004)

MA 12.5 Sa 10:00 TU EMH225

High-field magnetic susceptibility of ferromagnetic metals and alloys — •Sergey Mankovsky and Hubert Ebert — Dept. Chemie und Biochemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany

The results of a theoretical study of the high-field magnetic susceptibility of ferromagnetic metals and alloys are presented. The theoretical description of the magnetic susceptibility is based on a combination of a linear response approach and the fully relativistic Green's function formalism. In contrast to the paramagnetic state, additional contributions to the magnetic susceptibility (e.g. spin-charge response function, contributions related to a Fermi level shift) become important in the ferromagnetic state. These contributions have been taken into account in our calculations as well as the contribution of the Landau susceptibility. The results of calculations of the high-field susceptibility of the 3d transition metals Fe, Ni and Co are found in good agreement with experiment. Also the high-field susceptibilities calculated for binary Fe_xCo_{1-x}, Fe_xNi_{1-x}, Ni_xCu_{1-x} alloys are presented and compared with experimental data.

MA 12.6 Sa 10:15 TU EMH225

Accountig for many-body correlation effects in the calculations of the x-ray photoemission and magneto-optical properties of transition metals — •Stanislav Chadov, Jan Minar, Alexander Perlov, and Hubert Ebert — Department Chemie, University of Munich, Butenandstr. 5-13, D-81377 Munich, Germany

Calculations of valence band photoemission spectra on the basis of the LDA have been very succesfull in the past for many transition metal systems. However it is well known that correlation effects play for some materials a rather crucial role. Fortunately, it is often well justified to represent these by a local (site-diagonal) self-energy. In this case correlation effects can straightforwardly be incorporated within calculations based on the one-step model of photoemission. This applies in particular for its spin-polarised relativistic version that allows to deal with the Fano-effect and magnetic dichroism. Corresponding results will be presented for transition metal systems, for which the pure Fano-effect, that means the spin-polarisation of the photo-current due to spin-orbit coupling has been investigated. Results of investigations on the spontanous spin-polarisation in the ground-state by means of spin-resolved VB-XPS will be presented for the half-metallic ferromagnet NiMnSb. In addition, influence of correlation effects on the magneto-optical properties of Fe, Co and Ni will be presented. Within these investigations correlation effects are accounted for via the self-energy calculated by the recently proposed LDA+DMFT scheme (dynamical mean field theory). As it turns out, taking correlation effects into account the agreement between theory and experiment is significantly improved.

MA 12.7 Sa 10:30 TU EMH225

Multiple scattering formalism for correlated systems: A KKR+DMFT approach — •Ján Minár[1], L. Chioncel[2], A. Perlov[1], H. Ebert[1], M.I. Katsnelson[2] und A.I. Lichtenstein[3] — [1]Dep. Chemie, LMU, Butenandtstr. 5-13, 81377 München, Germany — [2]University of Nijmegen, NL-6525 ED Nijmegen, The Netherlands — [3]Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany

We present a charge and self-energy self-consistent computational scheme for correlated systems based on the Korringa-Kohn-Rostoker (KKR) multiple scattering theory with the many-body effects described by the means of dynamical mean field theory (DMFT). The corresponding local multi-orbital and energy dependent self-energy is included into the set of radial differential equations for the single-site wave functions. The Green's function is written in terms of the multiple scattering path operator, the later one being evaluated using the single-site solution for the t-matrix that in turn is determined by the wave functions. An appealing feature of this approach is that it allows to consider local quantum and disorder fluctuations on the same footing. Within the Coherent Potential Approximation (CPA) the correlated atoms are placed into a combined effective medium determined by the dynamical mean field theory (DMFT) self-consistency condition. Results of corresponding calculations for pure Fe, Ni and Fe_xNi_{1-x} alloys are presented.