

Relativistic and correlation effects in magnetic solids

H. Ebert, J. Minar, S. Chadov and A. Perlov

Department Chemistry / Physical Chemistry
University of Munich, Germany

The interplay of magnetic ordering and spin-orbit coupling leads to a large variety of phenomena that are even of great technological importance. Corresponding well known examples are the magneto-crystalline anisotropy or orbital contributions to the magnetic moments and hyperfine fields. As a peculiar spin-orbit induced ground state property one may add the occurrence of a field gradient in cubic ferromagnets. Besides the galvano-magnetic effects spin-orbit coupling in addition gives rise to many interesting effects in electron spectroscopy. A theoretical approach is presented that allows a detailed investigation of these spin-orbit induced phenomena in magnetic solids. This is achieved by using the spin-polarized relativistic version of multiple scattering or Korringa-Kohn-Rostoker (SPR-KKR) formalism on the basis of local spin density functional theory (LSDA). Corresponding applications to a variety of transition metal bulk, surface and cluster systems will be presented. To allow for a more detailed discussion of the results a simplified analytical approach will be used. As LSDA turns out to provide often an insufficient basis -in particular when dealing with magnetic properties connected with the orbital degree of freedom of an electron- various schemes that are designed to allow for an improved treatment of correlation effects will be presented together with corresponding results.