Correlation effects in transition metal nano-systems treated by means of the LSDA+DMFT scheme

Hubert Ebert[1], Jan Minar[1,3], Svitlana Polesya[1], Sergiy Mankovskyy[1], and Ondrej Sipr[2]

[1]*University Munich, Dept. Chemistry, Butenandtstr. 5-13, Munich, Germany*
[2]*Institute of Physics, Academy of Sciences of the Czech Republik, Praha, Czech Republic*
[3]*New Technologies-Research Center, University of West Bohemia, Pilsen, Czech Republic*

The combination of local spin density approximation (LSDA) and the dynamical mean field theory (DMFT) provides a very powerful basis to treat correlations beyond plain LSDA. A fully self consistent implementation on the basis of the multiple scattering Green function formalism (KKR-GF) allows in particular to investigate the impact of correlation effects for nano-systems. In addition, the use of a fully-relativistic formulation permits to study spin-orbit-induced properties. This platform is used for an investigation of various transition metal surface systems. The first part of the contribution deals with the magnetic properties of the surfaces of the pure ferromagnets Fe, Co and Ni and some magnetic surface films, while the second part of the talk is devoted to deposited magnetic clusters on non-magnetic substrates. The focus will be in particular on the influence of correlation effects on the spin-orbit induced magntic moments and spectroscopic properties. Accordingly, the corresponding LSDA+DMFT-based results are compared to those obtained using the LSDA and (in some few cases) the LSDA+U method.