Realistic DMFT calculations

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Density functional theory within the local density approximation (LDA) describe well the ground state structural properties but not the spectroscopy of strongly correlated magnetic materials with transition or rare-earth elements. Dynamical mean field theory (DMFT) in combination with the first-principle LDA-scheme (LDA+DMFT) is an efficient starting point to go beyond static density functional approximation and include effects of spin and orbital fluctuations in the local self-energy correction. Linear (LMTO) and N-th order (NMTO) muffin-tin orbitals present an natural basis for realistic many-body calculations in solids. Different correlated electron problems such as ferromagnetic transition metals and complex oxides will be discussed. Possibilities to includes the general multiorbital interaction vertex in the DMFT calculations within the continuous time QMC scheme as well as k-dependence approximation beyond DMFT will be addressed.