Authors:
Jörg Bünemann, Werner Weber, Florian Gebhard

Title:
Spin-orbit coupling in itinerant ferromagnets

Abstract:
The multi-band Gutzwiller method has been further generalized to incorporate the spin-orbit coupling in an open d or f shell. As a result, the hopping reduction factors are now tensors leading to spin-flip hopping in the effective single particle Hamiltonian. In addition, the atomic eigenstates of an open d-shell enter the variational scheme not only through their occupancies ($\approx$ 1000 variational parameters) but also through coupling amplitudes between these states (further $\approx$ 3000 variational parameters in the case of Iron). We report results of studies on Iron and Nickel which
a) yield the quasi-particle bands as observed in photoemission data,
b) reproduce the experimental values of the orbital moments and the magnetic anisotropy energy
c) for Nickel confirm Gersdorf's observation of a Fermi-surface topology change depending on the magnetic moment direction.