A new QSGW+DMFT approach applied to Ni

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We present a new approach to merging Quasiparticle Self-Consistent GW (QSGW) and dynamical mean field theory (DMFT), and apply it to Ni. While Fe is very well described in the Fermi liquid regime by QSGW alone, Ni is not. Most important, the exchange splitting is too large, because spin fluctuations are not accounted for. To include them we develop a novel form of QSGW+DMFT where DMFT modifies the self-energy in the spin channel only. This approach avoids double-counting problems. We also present an empirical method to include spin fluctions in QSGW by introducing an auxiliary effective magnetic field. Remarkable agreement is obtained with experiments by using our new methodology.

The method works well because QSGW contains nonlocality. In addition to spatial nonlocality the energy dependence of the self-energy is folded into a static hamiltonian through the QSGW construction. There is no "many-body" mass renormalization in Fe or Ni.