Role of local correlation effects in bcc Fe, hcp Co, and Mn doped GaAs.

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The strength of local electronic correlation effects in the spin-dependent electronic structure of ferromagnetic bcc Fe and hcp Co has been investigated by means of the LDA+DMFT (local density approximation combined with the dynamical mean-field theory) scheme, and compared with spin and angle-resolved photoemission spectroscopy. Although strong improvements are seen with respect to standard one-particle theory, still a perfect quantitative agreement cannot be reached. In particular strong differences are found between the quasiparticle lifetimes and the corresponding linewidths of the experimental spectrum. These differences cannot be explained as non-electronic contributions, and are shown to be stronger for Fe and weaker for Co, suggesting that they become weaker with increasing of the atomic number. A possible explanation can come from the neglected non-local correlation effects, as pointed out by recent experimental studies.

Finally preliminary results on the application of the LDA+DMFT scheme to the dilute magnetic semiconductor Mn doped GaAs are presented. The spectral and magnetic properties of this material are calculated for several different dopings, and compared with standard *ab-initio* simulations by means of density-functional theory.