Kondo physics and Hund's rule coupling in transition metal impurity systems

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We study the electronic structure of transition metal impurities (Mn, Fe, Co, Ni) in metallic hosts by combining density functional theory, many body impurity models and photoemission spectroscopy. While Mn and Co can be understood in terms of generalized Kondo models, Fe is shown to host sizable charge fluctuations and magnetic moments at the same time. In the latter case, there are no more well quantized magnetic moment and electronic correlations are largely driven by Hund's exchange J instead of Hubbard U. Fe in metal hosts realizes thus the single impurity limit of a Hund's metal. For this case, the dependence of the electronic excitation spectra and thermodynamic ground-state properties on hybridization between impurity and its surrounding is investigated systematically. Atomic multiplet peaks and exchange split many body satellites persist despite strong charge fluctuations and spin-freezing is observed.