Correlated electronic structure in LDA+DMFT: from transition metal oxides to rare earth compounds

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In the last decade the combination of dynamical mean-field theory (DMFT) with density functional theory in local density approximation (LDA) has emerged as one of the most powerful methods to study the electronic structure of strongly correlated materials. In this talk I will present the details of a LDA+DMFT implementation based on a full-potential linear muffin-tin orbital method (FP-LMTO). The construction of an appropriate set of local orbitals and the applicability of different impurity solvers such as Hubbard I, exact diagonalisation and SPTF will be discussed with a few examples. First, the ground state and spectral properties of SrRuO3 will be analysed, in order to understand the role of the local correlation effects on the itinerant 4d states of Ru. Then, the high degree of localization of the 4f-states in rare earth elements and compounds, e.g. TbN or Ce-pnictides, will be discussed. It will be shown that the Hubbard I approximation can give an excellent description of the most important physical properties. Finally the versatility of the exact diagonalization solver will be illustrated through the understanding of the electronic structure of the transition metal monoxides and Mn doped GaAs.