

From LDA+U to realistic correlated calculations

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We discuss a prospect of realistic electronic structure calculations with constrained screened Coulomb and Exchange interactions. Dynamical mean field theory in combination with the first-principle DFT-scheme is an optimal starting point to go beyond static density functional approximation and include effects of spin and charge fluctuations in strongly correlated materials. In order to go beyond the local approximation we used a dual-fermion/boson framework and shows that one can incorporate realistic Coulomb and Exchange interactions in electronic structure of correlated materials.