MAR06-2005-007233

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

First-principles calculations of electronic structure and spectra of strongly correlated systems: the LDA+U method

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Realistic approach to the electronic structure of complex materials which contains correlated d- or f- electrons will be discussed. The density functional theory within the local spin density approximation have been highly successful for electronic structure calculations and zero temperature magnetic properties of non-correlated systems. We investigate some failures of the LDA-scheme for the charge, spin and orbital ordering in transition metal compounds. General formulation of the LDA+U method which takes into account local Coulomb correlations for the d-shell of transition metals ions in the crystal within the mean-field approximation will be presented. The LDA+U scheme describe well the antiferromagnetic Mott insulators, rare-earth and actinide systems. Electronic structure, spin and orbital moments and lattice distortions of transition-metal compounds are investigated in the framework of rotationally invariant LDA+U method. Starting from conventional LDA+U scheme the different ways to go beyond the mean-field approximation which includes in effects of the spin- and charge-fluctuations will be analyzed. Dynamical mean field theory (DMFT) in combination with the first-principle LDA scheme (LDA+DMFT) is a good starting point for calculation of the quasiparticle spectrum for metallic transition metal systems. Recent progress in analysis of the metal-insulator transition for complex transition metal oxides and calculations of the spectral function for itinerant magnetic systems will be discussed.