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NiO - Dynamical Mean Field Study of Charge-Transfer Insulator J. KUNES, University of Augsburg, Germany, V.I. ANISIMOV, Institute of Metal Physics, Yekaterinburg, Russia, A.V. LUKOYANOV, Ural State Technical University, Yekaterinburg, Russia, D. VOLLHARDT, University of Augsburg, Germany — Charge-transfer (CT) Mott insulators present an important group of transition metal compounds which exhibit phenomena such as metal-insulator transitions or high temperature superconductivity. The location of ligand states between the interaction-split d bands leads to additional complexity, which requires a description beyond a simple Hubbard model. Using a combination of *ab initio* bandstructure and dynamical mean field theory we study the single particle spectrum of the prototypical CT insulator NiO. Including the O-p orbitals to the Hamiltonian we obtain good agreement with PES and BIS experiments. Notably we find d-peak at the top of the valence band, which cannot be described in static theories, but which is seen in experiment and was reproduced in many-body calculations on small clusters. Studying the effect of doping we find the added holes to occupy the ligand p orbitals despite large Ni-d spectral weight at the top of the valence band. Heavy hole doping leads to a significant reconstruction of the single-particle spectrum and filling of the CT gap. This is the first LDA+DMFT study of charge transfer systems, which includes the $p-d$ hybridization explicitly and is thus able to provide a full description of valence and conduction band spectra.

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