Abstract Submitted
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DFT+DMFT calculation of band gaps for the transition metal monoxides NiO, CoO, FeO and MnO.[1] LONG ZHANG, Department of Physics, University of Florida, Gainesville, Florida, USA, PETER STAAR, Institute for Theoretical Physics, ETH Zurich, Switzerland, ANTON KOZHEVNIKOV, Swiss National Supercomputing Centre, ETH Zurich, Switzerland, THOMAS SCHULTHESS, Institute for Theoretical Physics, ETH Zurich, Switzerland, HAI-PING CHENG, Department of Physics, University of Florida, Gainesville, Florida, USA — We report calculated spectral functions of the four late transition metal monoxides MnO, FeO, CoO and NiO in the paramagnetic phase. We used density functional theory (DFT) in combination with dynamic mean field theory (DMFT), which gives much better description of band gaps. Both projected Wannier orbitals and the on-site screened Coulomb interactions are obtained from DFT ground states to ensure consistency. Because of the p-d hybridization in these materials, we calculated Coulomb interactions for the dp model as well as the d-dp model using the cRPA method. With the standard fully localized limit double counting correction, we found that the d-dp model gives results in better agreement with experiments. This work was supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), under Contract No. DE-FG02-02ER45995.

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