Constrained Random Phase Approximation calculated Coulomb interactions for NiO, CoO, MnO, FeO

Abstract

We report calculation of the on-site Coulomb interaction matrix for the four transition metal monoxides MnO, FeO, CoO and NiO in their paramagnetic phase, by using the constrained Random Phase Approximation (cRPA) method implemented in a FLAPW code. The following DFT+DMFT calculations of the band gaps, using the cRPA calculated interaction, improved the DFT results and agreed with experimental values qualitatively.