The Effect of the Coulomb Repulsion and the Exchange Interaction on Spin Moment of MnO

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We have studied the effect of the on-site Coulomb repulsion $U$ and intra atomic d-d exchange interaction $J$ on the spin magnetic moment of MnO within the linear muffin-tin orbital (LMTO) method. The resulting spin magnetic moment of Mn²⁺ ions, the on-site Coulomb repulsion $U$ fixed, increased with increasing of exchange interaction $J$. Furthermore we focus on the spin magnetic moment $4.58\mu_B$, in agreement with the experimental. We found, the relation between $U$ and $J$, the exchange interaction $J$ slightly decreased about 0.24 with increasing about 1 eV of the Coulomb repulsion $U$.

REFERENCES