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First-principles Investigation of Ground State Magnetic Structure and Effective Exchange Interaction in $GaFeO_3$ MYUNG JOON HAN, Seoul National University, TAISUKE OZAKI, AIST-RICS, JAEJUN YU, Seoul National University — Among many multiferroic materials, $GaFeO_3$ has attracted much attention due to its large magnetoelectric effect and the unique magneto-electric, magneto-optic, and piezoelectric properties. We report our first-principles calculations on the electronic and magnetic structures of multiferroic $GaFeO_3$. Based on the LDA+U density-functional theory by employing a linear-combination-of-localized-pseudo-atomic orbitals (LCPAO) method, $GaFeO_3$ in its ideal structure is shown to be antiferromagnetic. Through calculations of effective exchange interactions among Fe atoms at either Ga or Fe sites in $GaFeO_3$, it is concluded that net magnetic moments observed in experiments may arise from the Fe substitution at the Ga sites. Total energy calculations show that the site disorder among Fe and Ga sites is quite feasible, which is consistent with experiments. Unquenched orbital magnetic moment of Fe is found to exist possibly due to the broken inversion symmetry at the Fe site with the distortion of surrounding oxygens. The calculated orbital magnetic moments are discussed in comparison with the results of recent X-ray magnetic circular dichroism measurement.

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