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Antiferromagnetic Structure and Magnetic Properties of FeO with GGA + U + SOC Study

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The magnetic stability and electronic properties of the FeO compound are investigated using the framework of an all-electron full-potential linearized augmented-plane wave (FP-LAPW) method within the generalized gradient (GGA) and GGA + U approximations. We locate the ground state to be of rhombohedrally distorted B1 structure with compression along [111] direction. The values for the band gap and magnetic moments obtained with this parameter-free first principles method are in good agreement with experimental data. Finally, we conclude that the treatment of the correlated electrons (GGA + U) approach with the inclusion of spin-orbit-coupling (SOC) is important for the correct description of this compound.

Keywords: TMMs (Transition Metals Monoxides), FeO, high pressure, DFT.