Band structure and density of states of antiferromagnetic and ferromagnetic iron(II) oxide by ab initio simulations[1] GABRIEL LEITAO, FIDELE TWAGIRAYEZU, Texas State University, PABLO D. BORGES, Universidade Federal de Viosa, LUISA SCOLFARO, WIM GEERTS, Texas State University — The Vienna ab-initio Simulation Package (VASP) and density functional theory (DFT) were used to determine the spin-polarized band structure and density of states (DOS) of iron(II) oxide (FeO), and partial DOS of each atom. FeO was simulated with a rock-salt crystal structure (Fm3m, No. 225) grown in the [111] direction, with a basis consisting two atoms of iron and two of oxygen. Two Fe atoms allowed for custom spin orientation to simulate both antiferromagnetic and ferromagnetic cases. Primary lattice vectors were chosen with rhombohedral symmetry in order to simulate unit cell growth along the [111] direction. Multiple runs of VASP code were performed to determine optimal INCAR parameters, producing the band structure of FeO for two different paths of high-symmetry points, F-G-T-L-Γ and G-L-K-T-G, each showing 20 energy bands filled out with all the electrons in the system. GGA calculations resulted in band structures with a band gap of 0.0 eV, showing a metallic character for FeO. Since the band gaps are known not to be well determined using DFT, a GGA+U calculation was executed using U value of 3.0 eV for Fe atoms, and 0.0 eV for O, to open up the band gap to about 1.9 eV, as determined from previous ab initio studies.

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