American Mineralogist, Volume 88, pages 257–261, 2003

Structure, metal-insulator transitions, and magnetic properties of FeO at high pressures

STEPHEN A. GRAMSCH,[1,*] RONALD E. COHEN,[1] AND SERGEJ YU SAVRASOV[2]

[1]Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road NW, Washington, D.C. 20015, U.S.A.
[2]Department of Physics, New Jersey Institute of Technology, 161 Warren Road, Newark, New Jersey 07102, U.S.A.

ABSTRACT

The high-pressure behavior of rocksalt-structured FeO has been investigated using the LDA + U method, a first-principles computational technique that allows treatment of correlated electrons with strong localized repulsions. Within the local density approximation (LDA) FeO is predicted to be a metal, but with LDA + U, an insulating state is obtained at zero pressure. Electronic and magnetic behavior, the equation of state, and lattice strain are determined for three values of the Coulomb repulsion U. We find two self-consistent solutions, one with rhombohedral and one with monoclinic electronic symmetry. For U = 4.6 eV, the monoclinic solution becomes more stable than the rhombohedral solution at 110 GPa, leading to an insulator-metal transition; with increasing U, metallization occurs at higher pressures. Results from the LDA + U calculation suggest that the high-spin magnetic state should persist to pressures greater than 300 GPa. The method gives improved agreement with experiments for ground state properties as compared to LDA and GGA methods that do not explicitly include a local Coulomb repulsion.