The Ground State of FeO_2 under Lower-Mantle Conditions

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From the oxygen-rich atmosphere to the iron-rich core, the iron-oxygen (Fe-O) system spreads the entire pressure-temperature-composition range of our planet, iron oxides are important materials of Earth's interior, and play an important role in geological and biological processes. It is believed that under different pressures and temperatures, from the Earth's surface to the core, the electronic properties, oxidation states, spin states and magnetism of different iron oxides are distinctive. Recently, a pyrite-structured FeO_2 which has the lowest Fe/O compositional range to date [1] with a formal oxidation state of +4 was synthesized under the deep lower-mantle conditions. Here, we employed first-principle electronic structure calculations using different density functionals to investigate the electronic ground state at high pressures. For calculations using functionals including correction to the self-interaction, (i.e. Fock exchange), FeO_2 is found to be a ferromagnetic insulator with a formal oxidation state close to +2 at lower-mantle conditions. The Mossbauer isomer shift and high spin to low spin transition pressure are predicted. The theoretical information will help to characterize the electronic state of this novel material by experiments.

[1] Hu et al., (2016) *Nature* **534**, 241