Abstract Submitted
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Dynamical mean-field theory study of the high pressure behavior of FeO[1] A.C. KOLLIAS, R.E. COHEN, Carnegie Institution of Washington — First-principles calculations have an important part in the development of our understanding of Earth's interior, including geophysical and geochemical phenomena. Proper treatment of iron bearing minerals is fundamental in this respect. Unfortunately standard density functional theory (DFT) approaches such as the local density (LDA) or the generalized gradient approximations (GGA) fail in describing qualitative features of simple iron containing minerals; for example the insulating nature and magnetic structure of many metal oxides such as FeO. The LDA+U approximation, self-interaction correction (SIC), and dynamical mean-field theory (DMFT) have demonstrated significant improvement in the physical description of transition metal and rare earth compounds. Presented results will focus on theoretical predictions obtained with the DMFT method. The high pressure behavior and high-spin-low-spin phase transition for iron oxide in the distorted rocksalt (B1) structure.

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