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High Pressure Phase Transitions in FeO from Density Functional Theory, Quantum Monte Carlo and Dynamical Mean Field Theory LUKE SHULENBURGER, KEN ESLER, Geophysical Laboratory, Carnegie Institution, SERGEJ SAVRASOV, Department of Physics, University of California, Davis, JEONGNIM KIM, University of Illinois at Urbana-Champaign, R. E. COHEN, Geophysical Laboratory, Carnegie Institution — FeO has a rich behavior under pressure, exhibiting a structural phase transition as well as an insulator-metal transition and a spin collapse. The electronic transitions have been particularly difficult to explain because of the failure of Density Functional Theory (DFT) to capture the electronic state of FeO. We present results from three different methods to better understand the nature of this material. First, from DFT calculations we explore competing explanations for the spin collapse, finding that the increase in bandwidth is at least as important as the crystal field splitting. Additionally, we find that the ligand field effects are responsible for the majority of the change in the local energy levels on the Fe rather than the electrostatic crystal field effect. Secondly, we have performed Dynamical Mean Field Theory (DMFT) calculations. From these we find that the metal insulator transition involves the reorganization of the existing bands and not the appearance of new states at the Fermi level. Finally we test the validity of the approximate results obtained by DFT and DMFT by performing highly accurate Diffusion Monte Carlo calculations.

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