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Effects of pressure on the magnetic properties of FeO: A diffusion Monte Carlo study[1] JOSHUA TOWNSEND, LUKE SHULENBURGER, THOMAS MATTSSON, Sandia Natl Labs, KEN ESLER, Stone Ridge Technology, RONALD COHEN, Carnegie Institution of Washington — While simple in terms of structure and composition, both experimental and computational investigations have demonstrated that FeO has a rich phase diagram of structural phase transformations, electronic spin transitions, insulator-metal transitions, and magnetic ordering transitions, due to the open-shell occupation of the Fe 3d electrons. We investigated the magnetic and electronic structures of FeO under ambient and high pressure conditions using diffusion Quantum Monte Carlo (QMC) within the fixed-node approximation. QMC techniques are especially well suited to the study of strongly correlated systems because they explicitly include correlation into the ground-state wave function. Here we report on the effects of the choice of trial wave function on the ambient pressure lattice distortion due to AFM ordering, as well as the equation of state, spin collapse, and metal-insulator transitions.

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