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**Quantum Monte Carlo study of equilibrium phase stability of crystalline FeO** J. KOLORENC, L. MITAS, North Carolina State University, Raleigh, NC, A. KOLLIAS, K. ESLER, R. E. COHEN, Carnegie Institution of Washington, DC — We investigate phase stability of crystalline FeO at experimental equilibrium volume by means of several approaches. It is well known that energy ordering of the B1 (rocksalt) and the inverse B8 (NiAs) structures is reversed in standard DFT methods when compared to experiment. Therefore, we consider more advanced DFT-based band structure techniques, such as hybrid exchange-correlation functionals and LDA+U, and use the corresponding set of orbitals as an input for quantum Monte Carlo wave functions. We compare the results from these calculations and discuss the reasons for the DFT difficulties in describing the correct ground state of this solid.

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