

Abstract Submitted
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High Pressure Phase Transitions in FeO from Quantum Monte Carlo LUKE SHULENBURGER, R.E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, KEN ESLER, Department of Physics, University of Illinois at Urbana-Champaign, JEONGNIM KIM, National Center for Supercomputing Applications — LDA+U and LDA+DMFT are successful methods for determining the electronic structure of FeO under pressure, but they suffer from two deficiencies. The extreme sensitivity of the spin collapse in MnO on the parameters U and J casts doubt upon the predictive power of the methods¹. Additionally, the symmetry of the occupation matrix has a profound effect on the electronic structure and magnetoelastic coupling in FeO², and is not easy to determine a priori. We perform diffusion Monte Carlo (DMC) calculations for FeO at a range of pressures using trial wavefunctions generated with LDA+U for several values of U . The limits of the Slater-Jastrow wavefunction we use causes Variational Monte Carlo to give different and erroneous predictions of the optimal value of U , so we use the variational property of the nodal surface in DMC to find the optimal value. The magnetoelastic coupling is shown to be insensitive to the symmetry of the occupation matrix. Thus we are able to make an accurate prediction of the pressure for the high spin low-spin transition in FeO as the possibility of a ferromagnetic state at high pressures. ¹ Kasinathan, D. et al. *New J. Phys.* **9**, 235 (2007) ² Gramsch. S. A. et al. *American Mineralogist* **88**, 257 (2003)

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