Abstract Submitted
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Magnetic properties of FeO: a DFT+DMFT study[1] PENG ZHANG, Carnegie Institute of Washington, Washington D.C. 20015, R.E. COHEN, Geophysical Laboratory, Carnegie Institution, Washington, D.C. and Department of Earth Sciences, University College London, London, United Kingdom, KRISTJAN HAULE, Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA — The magnetic properties of the transition metal oxide FeO greatly effect its equation of state and elasticity, and thus have been of great interest [1-3]. But FeO is not treated well by density functional theory which makes it a metal, instead of an insulator at low pressures. Employing the newly developed method of the density functional theory plus dynamical mean field theory, the magnetic properties of FeO within a wide range of pressure and temperature are investigated. Relative to density functional theory, the local correlations of the Fe d-electrons is exactly included in the new method in a fully self-consistent way. Adopting the hybridization expansion continuous time quantum Monte Carlo method as the impurity solver, the ab initio calculated impurity magnetic susceptibility is inserted in the Bethe-Salpeter equation, to derive the bulk magnetic susceptibility. By exploring the antiferromagnetic ordering and the Neel temperature as a function of pressure and temperature, the magnetic phase diagram of FeO is plotted. Our preliminary results indicate $T_N = 203.091K$ at V=540 $b.a.u.^3$ and $T_N = 223.345K$ at V=520 $b.a.u.^3$.

[1] J. Badro et al, PRL, 83, 4101(1999). [2] M.P. Pasternak et al, PRL, 79, 5046 (1997). [3] A. Mattinla et al, PRL, 98, 196404(2007).

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