Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Insulator to Metal and Magnetic Transitions in FeO under High Pressure: DFT-DMFT Computations R.E. COHEN, Geophysical Laboratory, Carnegie Institution, KRISTJAN HAULE, GABI KOTLIAR, Rutgers University — We have applied DFT+Dynamical Mean Field Theory (DMFT) to FeO under varying pressure and strain to understand possible transitions in FeO. We use an LAPW basis set, and the lattice terms are evaluated using the WIEN2K LAPW code. The impurity model is solved using continuous time quantum Monte Carlo (CTQMC). Temperature enters explicitly, so we made special efforts to understand high temperature behavior relevant to geophysics. The computations are fully self-consistent, including the impurity levels and crystal field splitting, and the total energy is evaluated using the full potential and charge density of the lattice plus impurity models. We find with increasing pressure in paramagnetic FeO in a cubic lattice and U=8 eV a high-spin low-spin transition, with a possible intermediate spin state (characterized by intermediate occupancies of the t2g and eg states) between. We find that at 300K cubic FeO remains insulating to a factor of two compression (over 600 GPa). However, high temperatures (e.g. 2000K) and rhombohedral lattice strain promote a metal insulator transition. We are delineating the phase boundaries. This work is supported by NSF.

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Date submitted: 08 Dec 2010 Electronic form version 1.4