Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A DFT+DMFT study of magnetic properties of FeO at high pressure. PENG ZHANG[1], Department of Physics, Xi'An Jiaotong university Geophysical Laboratory, RONALD COHEN[2], Extreme Materials Initiative, Geophysical Laboratory, Carnegie Institution for Science, Washington, D.C. USA , K. HAULE, Department of Physics and Astronomy, Rutgers University, NJ, USA — FeO is an insulator with anti-ferromagnetic (AFM) spin ordering at ambient pressure. When external pressure is increased, the Néel temperature first increases at the pressure below 40 GPa. Experiments show the AFM ordering collapses at high pressures. Using the density functional theory plus dynamical mean-field theory (DFT+DMFT), we examined the nature of magnetic collapse of FeO and derived its magnetic phase diagram up to 180 Gpa. We found coexistence of high spin-low spin transition and paramagnetic-AFM transition, both driven by increased pressure. The high spin-low spin transition is result of partition and pairing of 3d electrons in iron. The local moment of iron atom after high spin-low spin transition is small but finite up to 180 GPa.

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Date submitted: 06 Nov 2015 Electronic form version 1.4