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**Metallization of FeO at High Temperatures and Pressures: DFT-DMFT Computations and Comparisons with Experiments** R.E. COHEN, Geophysical Laboratory, Carnegie Institution, KRISTJAN HAULE, Dept. Physics, Rutgers University — DFT+Dynamical Mean Field Theory (DMFT) was applied to FeO as a function of pressure and temperature. 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. 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 wide transition region between 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), except for a small region of high spin metal. However, at high temperatures (e.g. 2000K) a metallic state is found. We find excellent agreement with recent high temperature high pressure experiments (Ohta et al.). We are now studying the antiferromagnetic ordering and effects of lattice strain.

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