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Origin of Metallization of FeO at High Temperatures and Pressures from First-principles DFT-DMFT Computations R.E. COHEN, Geophysical Lab, Carnegie Institution, KRISTJAN HAULE, Dept. Phys., Rutgers Univ. — Experiments and theory show that FeO metallizes at high temperatures (∼2000K) and pressures (∼80 GPa) [1]. Here we use DFT+Dynamical Mean Field Theory (DMFT) with continuous time quantum Monte Carlo (CTQMC) to study the origin of the metallization. We find with increasing pressure in paramagnetic FeO in a cubic lattice 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 under compression. The metallization occurs from thermal fluctuations among different multiplets representing high- and low-spin states. We are now studying the AFM ground state, the Néel transition, and (Mg,Fe)O solid solutions. This work is supposed by NSF.

[1] Ohta, K., Cohen, R. E., Hirose, K., Haule, K., Shimizu, K. & Ohishi, Y. Experimental and Theoretical Evidence for Pressure-Induced Metallization in FeO with Rocksalt-Type Structure. Phys. Rev. Lett. 108, 026403 (2012).

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