Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Evolution of MnO under Pressure from Dynamical Mean Field Theory[1] WARREN E. PICKETT, KWAN-WOO LEE, RICHARD T. SCALETTAR, UC Davis, JAN KUNEŠ, Univ. of Augsburg, A.V. LUKOYANOV, Ural State Tech. Univ., Yekaterinburg, V.I. ANISIMOV, Inst. of Metal Physics, Yekaterinburg — Late transition metal oxides qualify as so called charge-transfer insulators whose description requires that the simple Hubbard interaction within the $3d$ orbitals has to be augmented by mixing with the ligand $2p$ states. MnO is a relatively simple realization (at ambient pressure) of such a system. Its pressure evolution at room temperature exhibits structural (B1–B8), magnetic (high spin – low spin) and electronic (insulator – metal) transitions, and correlated band theories[1] predict a S=5/2 to S=1/2 moment collapse. We report All-Electron + DMFT high-spin to low-spin or insulator to metal transitions, and a study of the paramagnetic fcc phase as volume is reduced, focusing on the behavior of the local magnetic moment and the metal-insulator transition. We also present single-particle excitation spectra that illuminate the character of the evolution.
[1]D. Kasinathan et al., Phys. Rev. B **74**, 195110 (2006)

[1]Supported by DOE Computational Materials Science Network.

Warren E. Pickett
UC Davis

Date submitted: 13 Dec 2006 Electronic form version 1.4