Evolution of MnO under Pressure from Dynamical Mean Field Theory$^1$ WARREN E. PICKETT, KWAN-WOO LEE, RICHARD T. SCALET-TAR, 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 3$d$ orbitals has to be augmented by mixing with the ligand 2$p$ 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.


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