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Unusual magnetic ground state in MnO under pressure. KLAUS KOEPERNIK, IFW Dresden, Germany, DEEPA KASINATHAN, MPI-CPfS, Dresden, Germany, WARREN E. PICKETT, Dept. of Physics, UC Davis, CA, USA — A study of the phase transitions in MnO under pressure is presented. The calculations are based on density functional theory. The onsite correlations in the Mn 3d shell are treated within the framework of LSDA+U. The major result is that the first phase transition (with increasing pressure), which is characterized by an isostructural magnetic moment collapse from spin 5/2 to spin 1/2, results in a low spin solution exhibiting an unexpected intra-atomic spin polarization pattern. An analysis of the influence of the symmetry, the magnetic ordering and the LSDA+U interactions shows that this unusual spin arrangement is the result of inter-orbital exchange terms. The dependence of the results on the parameters U and J will be discussed.

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