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Hybrid density functional study of Mott transition in MnO CRISTIAN V. DIACONU, RICHARD L. MARTIN, Los Alamos National Laboratory, IONUT D. PRODAN, GUSTAVO E. SCUSERIA, Rice University — The electronic structure, the magnetic moment and volume collapse of MnO under pressure is obtained from hybrid density functional theory using the recently developed screened hybrid exchange-correlation functional of Heyd, Scuseria and Ernzerhof (HSE). We study two crystal structures for MnO: cubic (rock salt) and hexagonal (nickel arsenide). We find two antiferromagnetic states for the NaCl structure: a high-spin state that couples two $S = 5/2$ moments, and a low-spin state that couples two $S = 1/2$ moments. At ambient pressure the high-spin state lies lowest. The low-spin phase becomes favored at a pressure of about 248 GPa, leading to a first order volume collapse. However, this transition is pre-empted by another first-order volume collapse at 178 GPa from the NaCl structure to a NiAs structure. This transition is predicted to be insulator to metal and is the realization of the Mott transition.

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