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LDA+U Picture of the Moment Collapse under Pressure in MnO

DEEPA KASINATHAN, J. KUNES, W. E. PICKETT, RICHARD. T. SCALETTAR, UC Davis, B. MADDOX, C.S. YOO, A.K. MCMAHAN, LLNL — The transition metal monoxide MnO crystallizes in the rock-salt structure and is a high-spin antiferromagnetic insulator at low temperatures. Under pressure, experimentally it is observed to undergo a metal-insulator transition along with a structural change to the nickel arsenide phase.[1,2,3] As the first step in a concerted effort to obtain a realistic theory of the pressure behavior of MnO, we have performed full potential local orbital (FPLO) LDA+U calculations in the rock-salt phase. The outcome is a first order moment collapse at reduced volume $V/V_0 \approx 0.73$, whereas within LDA the collapse is smoother and is centered around $V/V_0 \approx 0.68$. The moment collapse is from high spin 4.9 μ_B to a lower but nonzero spin value of 0.8 μ_B. The strong influence of symmetry-lowering (cubic to rhombohedral) by antiferromagnetism will be discussed. [1]. Kondo et al., J. App. Phys, 87, No.9, 4153 (2000) [2]. C.S. Yoo et al. (preprint 2004) [3]. Patterson et al., PR B 69, 220101 (2004)

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