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An Assessment of Hubbard U Corrections on Manganese Oxide Clusters ELISE Y. LI, Chemistry, Massachusetts Institute of Technology, DAVIDE CERESOLI, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Conventional density-functional approaches often fail in offering an accurate description of the spin-resolved energetics in transition metal complexes, due to spurious self-interaction errors (SIE). Previous studies have shown that a self-consistent DFT + U approach [1] can accurately correct SIE in TM complexes, providing excellent agreement with high-level quantum chemistry calculations. In this work we report a systematic evaluation of DFT + U in a series of small manganese oxide clusters (MnO_x, x=1-4) and their anions, focusing on structural, electronic and magnetic properties. It is found that DFT + U succeeds in systems where the valence electrons are essentially localized on the TM ion, but progressively worsens when the coordination number increases and more covalency comes into play between the TM center and neighboring atoms, pointing to the importance of choosing the appropriate correlated manifold when Hubbard corrections are added. [1] H. J. Kulik, M. Cococcioni, D. A. Scherlis, and N. Marzari, Phys. Rev. Lett., 2006, 97, 103001 .

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