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Accurate electronic-structure description of Mn complexes: a GGA+U approach ELISE Y. LI, Chemistry, Massachusetts Institute of Technology, HEATHER KULIK, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Conventional density-functional approach often fail in offering an accurate description of the spin-resolved energetics in transition metals complexes. We will focus here on Mn complexes, where many aspects of the molecular structure and the reaction mechanisms are still unresolved - most notably in the oxygen-evolving complex (OEC) of photosystem II and the manganese catalase (MC). We apply a self-consistent GGA + U approach [1], originally designed within the DFT framework for the treatment of strongly correlated materials, to describe the geometry, the electronic and the magnetic properties of various manganese oxide complexes, finding very good agreement with higher-order ab-initio calculations. In particular, the different oxidation states of dinuclear systems containing the $[Mn_2O_2]^{n+}$ (n= 2, 3, 4) core are investigated, in order to mimic the basic face unit of the OEC complex. [1]. H. J. Kulik, M. Cococcioni, D. A. Scherlis, N. Marzari, Phys. Rev. Lett., 2006, 97, 103001

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