Abstract Submitted
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Geometry and magnetic structure variation in manganese-oxide clusters determined by a self-consistent, LCAO method[1] KRISTEN WILLIAMS, US Army Research Lab, Aberdeen Proving Ground, MD 21005, JOSEPH HOOPER, Dept. of Physics, Naval Postgraduate School, Monterey, CA 93943 — *Ab initio* simulations are used to study the variation in geometry and magnetic structure in Mn_xO_y (x =3,4; y =1,2) clusters. The groundstate wavefunctions for clusters with different magnetic coupling (ferromagnetic, ferrimagnetic and antiferromagnetic) are modeled with linear combinations of atomic orbitals (LCAOs). Self-consistent energies for different spin isomers are calculated by constraining the magnetic moments of Mn atoms constituting each basis AO. The ferrimagnetic and antiferromagnetic ground-state structures of Mn_xO_y are 0.16–1.20 eV lower in energy than their ferromagnetic isomers. The presence of oxygen thus stabilizes low-spin isomers relative to the preferred high-spin ordering of bare Mn_3 and Mn_4. Each cluster has a preferred overall magnetic moment, and no evidence is seen of competing states with different spin multiplicities. However, non-degenerate isomags (clusters that possess the same spin multiplicity but different arrangements of local moments) do contribute to peak broadening observed in negative-ion photoelectron spectra. Proper accounting for all possible isomags is shown to be critical for accurate comparison with experimental spectra.

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