Abstract Submitted
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Electronic structure of Mn and Fe oxides WALTER HARRISON, Stanford University — We present a clear, simple tight-binding representation of the electronic structure and cohesive energy (energy of atomization) of MnO, Mn_2O_3, and MnO_2, in which the formal charge states Mn^{2+}, Mn^{3+}, and Mn^{4+}, respectively, occur. It is based upon localized cluster orbitals for each Mn and its six oxygen neighbors. This approach is fundamentally different from local-density theory (or LDA+U), and perhaps diametrically opposite to Dynamical Mean Field Theory. Electronic states were calculated self-consistently using existing parameters [1], but it is found that the charge *density* is quite insensitive to charge *state*, so that the starting parameters are adequate. The cohesive energy per Mn is dominated by the transfer of two s electrons to oxygen p states, the same for all three compounds. The differing transfer of majority d electrons to oxygen p states, and the coupling between them, accounts for the observed variation in cohesion in the series. The same description applies to the perovskites, such as $La_xSr_{1-x}MnO_3$, and can be used for FeO, Fe_2O_3 (and FeO_2), Because the formulation is local, it is equally applicable to impurities, defects and surfaces.

[1] Walter A. Harrison, *Elementary Electronic Structure,* World Scientific (Singapore, 1999), revised edition (2004).

Walter Harrison
Stanford University

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