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A few ways in which LDA et al can produce a wrong description of magnetism in oxides[1] ALEX ZUNGER, S. LANY, H. RAEBIGER, NREL — Part of the anarchy that exist in the literature regarding conflicting predictions of ferromagnetism in oxides can be attributed to problems in LDA and its application:(1) LDA et al tend to place the oxide conduction band minima CBM) at much too deep energies; transition-metal impurity levels then incorrectly appear within the (delocalized) LDA continuum (instead of in the gap). This leads to overly optimistic result of long -range magnetism. This is not fixable via LDA+U.(2) Oxides are naturally off-stoichiometric, exhibiting significant concentration of indigenous free-carriers that greatly affect the occupancy of impurity levels. Yet, such non-stoichiometry is ignored in many calculations using instead a perfect host crystals. This alters the magnetic properties. (3) LDA- Predicted magnetism in defected oxides without TM impurities often rely on the defect orbitals (e.g, cation vacancy) being equally delocalized over all of its ligand atoms. While inherent to LDA, experiment, as well as more correlated approaches reveal that such orbitals are "locked" instead onto a single ligand. This symmetry-breaking causes them to become too localized for (percolative) magnetism. We show here how such problems might be fixed.

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