Polymorphous band structure model of gapping in the antiferromagnetic and paramagnetic phases of the Mott insulators MnO, FeO, CoO, and NiO

Giancarlo Trimarchi,[1,*] Zhi Wang,[2] and Alex Zunger[2,*]
[1]Department of Chemistry, Northwestern University, Evanston, Illinois 60208, USA
[2]Renewable and Sustainable Energy Institute, University of Colorado, Boulder, Colorado 80309, USA

involving a distribution of transition metals, each with its own local environment. No mean-Þeld-embedding bath is needed, and no arbitrarily selected symmetry breaking is involved.

Our underlying conjecture is that time ßuctuations that could average the magnitude (not orientation) of the magnetic moment to zero would involve excitations across the band gap, so the time scale for such ßuctuations is slow in relation to the relevant electron energy scale. Thus the magnitude of the on-site moments $|\mu_i|^2$ in gapped PM systems will not be zero, deciding the higher energy scale of the problem. As a result, the time average of the gaps of all conÞgurations could be nonzero. Even though the average $P = \sum_n c_n P(\xi_i^{(n)})$ over the ensemble of microscopic spin conÞgurations is involved, the band gaps and moments $P(\xi_i^{(n)})$ of individual conÞgurations are nonzero.

Indeed, the fact that the antiferromagnetic ordering disappears at T_N does not mean that the magnetic moments at the transition metal sites go to zero too. On the contrary, the transition metal atoms retain robust local magnetic moments as evidenced by the Curie-Weiss behavior of the magnetic susceptibility as a function of the temperature. This means that the symmetry between spin-up and spin-down electronic states is instantaneously broken at each site thus allowing the localized magnetic moments to form. In contrast, in the naïve DFT nonmagnetic approximation to the PM spin conÞguration [4

FIG. 1. Percent fraction (n$_{NN}$

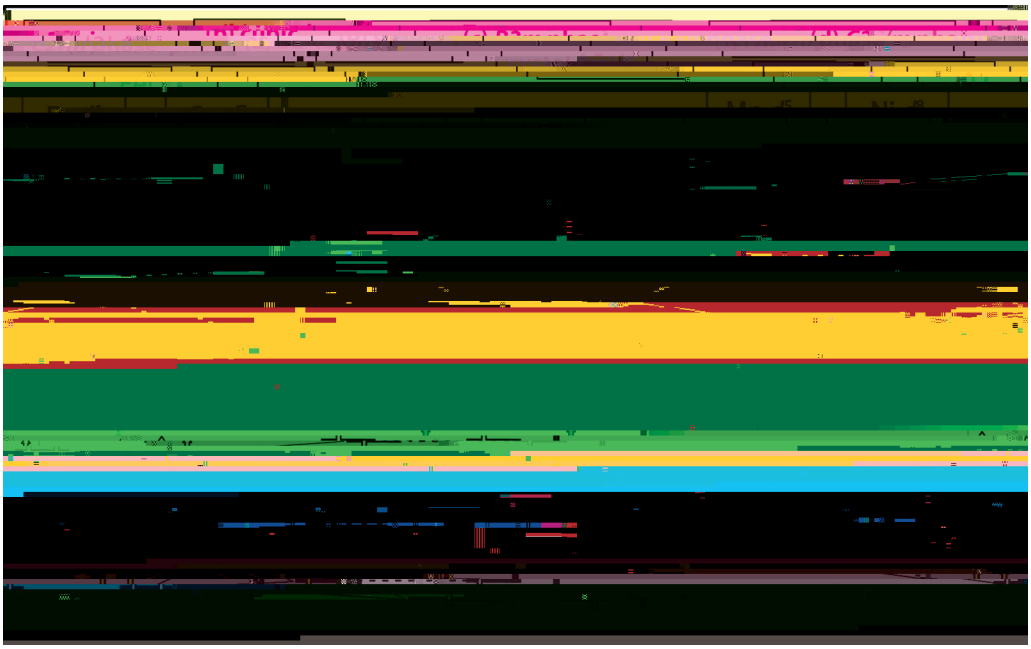

FIG. 2. Schematic of the sequence of level splittings and combinations for the d orbitals in MnO, NiO, FeO, and CoO as the exchange coupling and the crystal Þeld of the symmetry appropriate to each phase are progressively imposed: (a) splitting of the d orbitals into the

FIG. 3. Projected density of states (PDOS) on the transition metal d orbitals (t_{2g} and e_g components) calculated by DFT+U (U = 5 eV) for MnO and NiO in (a) and (b) the AFM phase with fully relaxed

FIG. 6. Minority-spin electron density (r) in the regions with positive magnetization m(r) = (r) Š (r) > 0 within the magnetic 64-atom SQS cell used in the DFT+U (U = 5 eV) calculations of the PM phases of (a) FeO and (b) CoO. To avoid visual clutter, we masked out the regions of space within spheres of of radius centered at the oxygen sites.

phases and of the splitting of these mixed orbitals that lifts the degeneracy of the unperturbed states. In PM FeO, (

D. Comparison with other approaches

Previously, the paramagnetic phases, including those of the

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