

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

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

Our underlying conjecture is that time fluctuations 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 fluctuations 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 configurations could be nonzero. Even though the average $\mu = \sum_n c_n \mu_i^{(n)}$ over the ensemble of microscopic spin configurations is involved, the band gaps and moments $\mu_i^{(n)}$ of individual configurations are nonzero.

Indeed, the fact that the antiferromagnetic ordering disappears \bar{m}_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 naive DFT nonmagnetic approximation to the PM spin configuration [4



FIG. 1. Percent fraction n_{NN}



FIG. 2. Schematic of the sequence of level splittings and combinations for orbitals in MnO, NiO, FeO, and CoO as the exchange coupling and the crystal field of the symmetry appropriate to each phase are progressively imposed: (a) splitting of the 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 $\rho(r)$ in the regions with positive magnetization $m(r) = \langle \tilde{S}(r) \rangle > 0$ 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 radius r_{mask} 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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