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Effect of the electron-phonon coupling on the magnetism in the Nickelatematerials $\mathbf{Li}_x\mathbf{Na}_{1-x}\mathbf{NiO}_2$ H. MESKINE, S. SATPATHY, University of Missouri-Columbia — The absence of magnetic and orbital ordering in the nickelate $LiNiO_2$ has long been a subject of speculation, especially in light of the fact that its sister compound $NaNiO_2$ exhibits both magnetic and orbital structure. Although this issue has attracted much attention in recent years from both the theoretical and experimental fronts, the unusual spin-glass state of lithium nickelate remains a mystery. We are able to account for the observed type A magnetic structure of $NaNiO_2$ by computing the intra- and inter-layer exchange couplings using a model Hamiltonian which includes electronic hopping, on- site energy, and Coulomb interaction. The electronic structure parameters are obtained via *ab initio* density functional theory calculations using the linear muffin-tin orbitals method. The dynamical electron-phonon coupling is then introduced by quantization of the motion of the Na/Li ion. We compute the ground-state of the full Hamiltonian by exact diagonalization as well as using a Lang-Firsov unitary transformation. We find that the coupling of the electronic degrees of freedom to the motion of the metallic ion decreases the exchange coupling.

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