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Charge disproportionation without charge transfer in the rare-earth nickelates as a possible mechanism for the metal-insulator transition STEVEN JOHNSTON, University of Tennessee, ANAMITRA MUKHERJEE, ILYA ELFIMOV, MONA BERCIU, GEORGE SAWATZKY, University of British Columbia — We study a model for the metal-insulator (MI) transition in the rare-earth nickelates $RNiO_3$, based upon a negative charge transfer energy and coupling to a rock-salt like lattice distortion of the NiO_6 octahedra. Using exact diagonalization and the Hartree-Fock approximation we demonstrate that electrons couple strongly to these distortions. For small distortions the system is metallic, with ground state of predominantly $d^8\,ligand$ character, where *ligand* denotes a ligand hole. For sufficiently large distortions ($\delta d_{\mathrm{Ni-O}} \sim 0.05 - 0.10$ Å), however, a gap opens at the Fermi energy as the system enters a periodically distorted state alternating along the three crystallographic axes, with $(d^8\,ligand^2)_{S=0}(d^8)_{S=1}$ character, where S is the total spin. Thus the MI transition may be viewed as being driven by an internal volume "collapse" where the NiO_6 octahedra with two ligand holes shrink around their central Ni, while the remaining octahedra expand accordingly, resulting in the superstructure observed in x-ray diffraction in the insulating phase. This insulating state is an example of charge ordering achieved without any actual movement of the charge, similar to that reported in a prior DMFT study.

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