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Low-energy description of rare-earth nickelates OLEG PEIL, University of Geneva, ALASKA SUBEDI, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, ANTOINE GEORGES, College de France, Paris
— We propose a simple low-energy theory of rare-earth nickelates that involves only two e_g orbitals per nickel site. We show that this theory, in particular, captures all important features of the metal-insulator transition of nickelates. In the monoclinic insulating state, bond-length disproportionation splits the manifold of e_g bands, leading to a modulation of the effective on-site energy. We show that, when subject to a local Coulomb repulsion U and Hund's coupling J, the resulting bond-disproportionated state is a paramagnetic insulator for a wide range of interaction parameters. Furthermore, we find that when $U - 3J$ is small or negative, a spontaneous instability to bond disproportionation takes place for large enough J. In the metallic phase, on the other hand, this negative effective coupling results in the suppression of the orbital polarization of e_g states, consistent with experiments and earlier calculations. This minimal theory emphasizes that a small or negative charge-transfer energy, a large Hund's coupling, and a strong coupling to bond-disproportionation are the key factors determining the physics of nickelates. Finally, we discuss particular experimental consequences of this theoretical picture.

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