A low-energy description of rare-earth nickelates

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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 captures all important features of nickelates, such as the metal-insulator transition in small-cation nickelates and a rather moderate orbital polarization in heterostructures based on LaNiO₃. In particular, we show that the bond-disproportionated state of the low-temperature monoclinic phase, when subject to local Coulomb repulsion $U$ and Hund's coupling $J$, is a paramagnetic insulator in a wide range of interaction parameters. Furthermore, we find that in the high-temperature orthorhombic phase a spontaneous instability to bond disproportionation takes place for large enough $J$ when $U-3j$ is small or negative. In the metallic phase, on the other hand, this negative effective coupling results in the suppression of the orbital polarization, consistent with experiments. 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. Importantly, this theoretical picture suggests a number of particular experimental consequences, such as a peculiar behavior of the optical conductivity in the insulating state, which is nicely confirmed by optical spectroscopy experiments.