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.