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Total energy calculations of correlated electron compounds: theory and application to rare earth nickelates[1] HYOWON PARK, Department of Applied Physics and Applied Mathematics & Department of Physics, Columbia University, ANDREW MILLIS, Department of Physics, Columbia University, CHRIS MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — We use density functional theory (DFT) plus dynamical mean field theory (DMFT) method, along with DFT+U and Hartree-Fock methods to compute the electronic energy as a function of crystal structure for rare earth nickelates. We show that full charge self-consistency can be essential for obtaining qualitative agreement with experiment and that the choice of double counting correction has an important effect on the energy. Furthermore, the precise definition (projector vs Wannier) of the correlated d-orbitals has a minimal effect. We show that charge self-consistent DFT+DMFT, as opposed to DFT+U, is critical to describing the magnetic-insulator to paramagnetic-metal phase boundary in the rare earth nickelate phase diagram.

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