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【602】 Breathing mode distortion and magnetic order in rare-earth nickelates $R\text{NiO}_3$

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Perovskite rare-earth nickelates, $R\text{NiO}_3$, display a rich and only partially understood phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT) that is accompanied by a structural distortion. We use density functional theory (DFT) and its extensions (DFT+U, DFT+DMFT), combined with symmetry-based distortion mode analysis to explore the interplay between lattice distortions, magnetic order, and electronic correlation effects in rare-earth nickelates. Thereby, we want to explore the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom.

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