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[602] Breathing mode distortion and magnetic order in rare-earth nickelates $RNiO_3$

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Perovskite rare-earth nickelates, RNiO₃, 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.

Authors: HAMPEL, Alexander (ETHZ - ETH Zurich); Prof. EDERER, Claude (ETH Zurich)

Presenter: HAMPEL, Alexander (ETHZ - ETH Zurich)

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