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Invitation
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Structurally Triggered Metal-Insulator Transition in Rare-Earth Nickelates.

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Abstract:
Rare-earth nickelates form an intriguing series of correlated perovskite oxides. Apart from LaNiO3, they exhibit on cooling a sharp metal-insulator electronic phase transition, a concurrent structural phase transition and a magnetic phase transition toward an unusual antiferromagnetic spin order. Appealing for various applications, full exploitation of these compounds is still hampered by the lack of global understanding of the interplay between their electronic, structural and magnetic properties. Here, we show from first-principles calculations that the metal-insulator transition of nickelates arises from the softening of an oxygen breathing distortion, structurally triggered by oxygen-octahedra rotation motions. The origin of such a rare triggered mechanism is traced back in their electronic and magnetic properties, providing a united picture. We further develop a Landau model accounting for the evolution of the metal-insulator transition in terms of the R cations and rationalising how to tune this transition by acting on oxygen rotation motions.

Alain Mercy, Jordan Bieder, Jorge Iñiguez and Philippe Ghosez,
https://arxiv.org/abs/1709.07240

M. Medarde, 3283