

Revealing the electronic ground state of ReNiO_3 combining high-resolution Ni-L₃ X-ray absorption and resonant inelastic X-ray scattering

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Perovskite rare-earth (Re) nickelates ReNiO_3 continue to attract a lot of interest thanks to their intriguing physical properties like sharp metal to insulator transition (MIT), unusual magnetic order [1] and expected superconductivity in nickelate-based heterostructures [2]. Full understanding of these materials, however, is hampered by the difficulties in describing their electronic ground state (GS).

Taking a NdNiO_3 thin film as a representative example, we reveal with x-ray absorption (XAS) and resonant inelastic x-ray scattering (RIXS) an unusual coexistence of bound and continuum excitations providing a strong evidence for the abundance of O 2p holes in the GS of these materials. Using an Anderson impurity model interpretation, we show that these distinct spectral signatures arise from a Ni $3d^8$ configuration along with holes in the O 2p valence band, confirming suggestions that these materials do not obey a “conventional” positive charge-transfer picture, but instead exhibit a negative charge-transfer energy, with O 2p states extending across the Fermi level [3].

References

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