Revealing the electronic ground state of ReNiO$_3$ combining Ni-L$_3$ x-ray absorption and resonant inelastic x-ray scattering

VALENTINA BISOGNI, Brookhaven National Laboratory, New York, SARA CATALANO, University of Geneva, Switzerland, ROBERT GREEN, University of British Columbia, Canada, MARTA GIBERT, RAOUl SCHERWITZL, University of Geneva, Switzerland, YAOBO HUANG, Paul Scherrer Institute, Switzerland, SHADI BALANDESH, University of British Columbia, Canada, VLADIMIR N. STROCOV, Paul Scherrer Institute, Switzerland, PAVLO ZUBKO, University of Geneva, Switzerland, GEORGE SAWATZKY, University of British Columbia, Canada, JEAN-MARC TRISCONE, University of Geneva, Switzerland, THORSTEN SCHMITT, Paul Scherrer Institute, Switzerland — Rare-earth nickelates ReNiO$_3$ attract a lot of interest thanks to their intriguing physical properties like sharp metal to insulator transition, unusual magnetic order and expected superconductivity in nickelate-based heterostructures. 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 and resonant inelastic x-ray scattering unusual coexistence of bound and continuum excitations, providing strong evidence for abundant 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 exhibit a negative charge-transfer energy, with O 2p states extending across the Fermi level.

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