

Abstract Submitted
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Non-Resonant Inelastic X-Ray Scattering and Energy-Resolved Wannier Function Investigation of $d-d$ Excitations in NiO and CoO¹ B.C. LARSON, J.Z. TISCHLER, Oak Ridge National Lab., P. ZSCHACK, APS, WEI KU, Brookhaven National Lab., C.C. LEE, Tamkang Univ. — We have investigated dipole-forbidden $d-d$ excitations in the non-resonant inelastic x-ray scattering (NIXS) spectra of NiO and CoO. The spectral weight of these Mott-gap excitations vanishes at small q , but dominates the large- q NIXS spectra and is highly anisotropic with well-defined nodal directions. Theoretical analyses based on energy-resolved Wannier functions within LDA+ U have shown the origin of the anisotropy to be selection-rules reflecting the underlying cubic point group symmetry. The measured and calculated orientation anisotropies of the NIXS spectra will be discussed and the anisotropies for NiO and CoO will be compared to demonstrate that such measurements represent sensitive probes of weak symmetry breaking in particle-hole wave functions.

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