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Non-resonant Inelastic X-Ray Scattering and Energy-Resolved Wannier Function Investigation of Local Excitations in Transition Metal Monoxides NiO and CoO B.C. LARSON, J.Z. TISCHLER, ORNL, WEI KU, BNL and SUNY, Stoney Brook, CHII-CHENG LEE, Tamkang Univ. Taiwan, OSCAR RESTREPO, Univ. TN, Knoxville, A.G. EGUILUZ, Univ. TN, Knoxville and ORNL, P. ZSCHACK, FS-MRL UIUC, K.D. FINKELSTEIN, CHESS, Cornell Univ. — Non-resonant inelastic x-ray scattering (NIXS) and energy- resolved Wannier function analysis have been used to probe the strongly correlated electronic structure of NiO and CoO. NIXS measurements of the dynamical structure factor s(q,w) as a function of momentum transfer q and frequency w have shown that dipole-forbidden, d-d excitations appear within the optical gap for large wavevectors ($q > 2/A$), become the dominant structure in the loss spectra for $q > 3/A$, and reach a maximum at $q \sim 7/A$. In contrast to the loss-spectra observed in resonant-probe studies of NiO and CoO, non-resonant spectra show only two excitations that are highly anisotropic - strongest in the [111] direction and weakest (or missing) in the [001] direction. Energy-resolved Wannier function analyses of vertex matrix elements within LDA+U demonstrate that the anisotropy provides a sensitive measure of electronic symmetry-breaking in these atomic-like d-d excitations as a result of point-group symmetry selection rules.

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