Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Sorting Category: 03.4 (E)

Investigation of Dipole-Forbidden $d-d$ Excitations in Strongly Correlated Transition-Metal Oxides Using Higher-Order Multipole, Non-resonant Inelastic X-Ray Scattering[1]

B.C. LARSON, J.Z. TISCHLER, ORNL, C.-L. YEH, Tamkang Univ., Taiwan, C.-C. LEE, WEI KU, BNL — We have shown that quadrupole and higher order multipole non-resonant inelastic x-ray scattering (NIXS) at large wavevectors, q, provides direct access to dipole-forbidden $d-d$ excitations (Larson et al. *Phys. Rev. Lett.* **99**, 026401 (2007)). NIXS measurements using the XOR/UNI beamline at the APS have shown that the large-$q$intensity of on-site excitons in NiO and CoO is highly anisotropic in q and dominates the energy loss spectrum. Energy-resolved Wannier function analyses have shown that the anisotropies, including a nodal direction for NiO, provide direct information on the point-group symmetry of the particle-hole wave functions for transition-metal oxides. The interpretation of these large-q NIXS measurements will be discussed in connection with energy-resolved Wannier function analyses and LDA+U dynamical response calculations. Implications for the extension of such investigations to manganite systems will be considered.

[1]Research sponsored by the DOE-BES Division of Materials Sciences and Engineering; the APS is supported by the DOE Office of Science.

[X] Prefer Oral Session
[ ] Prefer Poster Session

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Date submitted: 11 Dec 2007 Electronic form version 1.4