

Abstract Submitted
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The Dynamical Structure Factor of NiO and CoO* B.C. LARSON, J.Z. TISCHLER, ORNL, P. ZSCHACK, UNICAT-UIUC-FSMRL, K.D. FINKELSTEIN, CHESS-Cornell, WEI KU, BNL, O. RESTREPO, U-Tenn., A.G. EQUILUZ, U-Tenn. and ORNL — Non-resonant inelastic x-ray scattering (IXS) and *ab initio* dynamical electronic response calculations have been used to investigate highly correlated transition metal monoxides NiO and CoO. Absolute IXS measurements were made as a function of the magnitude and orientation of momentum transfers, q , at the APS and CHESS using energy resolution ranging from 0.3 – 1.1 eV. In addition to ~ 4 eV energy gaps observed for all q , sharp excitonic peaks were observed below the gap of both NiO and CoO for momentum transfers higher than $\sim 2 \text{ \AA}^{-1}$. Comparisons of $S(q,w)$ measurements with dynamical response calculations performed within LDA+U (including crystal field effects) show that the gap energy and the electronic response above the gap are described by $U \sim 8$ eV within RPA for low q -values. However, the excitonic peaks are not described by LDA+U calculations, nor are the calculated $S(q,w)$ spectra in agreement with the measured response for large q . The results will be compared with resonant x-ray emission and resonant electron energy loss spectra in the literature. *Work at the APS supported by the DOE Office of Science, DMS under contract with ORNL, managed by UT-Battelle, LLC; UNI-CAT is supported by UIUC, ORNL, NIST and UOP Res., Inc. The APS is supported by the DOE and CHESS is supported by the NSF.

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