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Inelastic X-Ray Scattering Investigations of Electronic Correlations in Transition-Metals and Transition-Metal Oxides

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The high brilliance of 3rd generation synchrotron sources has made non-resonant inelastic x-ray scattering (IXS) measurements of the energy-loss spectra in transition-metals and transition-metal compounds routine when the ~1 eV energy resolution of the high heat-load Si monochromator is adequate. We have combined 1 eV energy resolution IXS measurements on the UNICAT ID-33 beamline with first principles all-electron dynamical electronic response calculations to investigate electronic correlations including crystal local-field and many-body local-field effects in a series of transition-metals and transition-metal oxides. Direct comparisons of first-principles calculations of the dynamical structure factor with absolute IXS measurements as a function of wave vector and energy loss on Sc, Cr, TiO2, NiO, and CoO will be used to illustrate the ability to extract spectroscopic information on d-d transitions, crystal local field effects, novel collective modes, and coulomb repulsion potentials in these materials. The method used for absolute calibration of IXS for arbitrary materials and the method used for the removal of quasi-elastic tails will be discussed.

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