

Abstract Submitted
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Real-space Green's function calculations of valence Compton profiles for Nonresonant Inelastic X-ray Scattering¹ BRIAN MATTERN, JOSHUA KAS, JOHN REHR, U. Washington — Nonresonant inelastic x-ray scattering (NIXS) from core- and semi-core shells at 50-1000 eV binding energies is an emerging field of synchrotron light source science, with applications in high pressure science, electrical energy storage, f-electron materials, and catalysis, etc. In such experiments, the Compton scattering of x-rays by valence electrons produces a significant background signal that spans the energy loss range of interest for NIXS. Thus, first-principles theoretical calculations of the double-differential cross-section for Compton scattering in the energy loss and momentum transfer ranges of interest are needed to account for this background. Here, we report an approach using a real space Green's function method to calculate the valence Compton profile in the impulse approximation. Illustrative calculations are presented and compared with experiment.

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