

First-principles Calculations of Resonant Inelastic X-ray Scattering

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Resonant inelastic X-ray scattering (RIXS) probes a variety of low energy excitations with fine experimental control. In addition to traditional techniques, such as inelastic neutron scattering and angle resolved photoemission, RIXS has become an important, high precision characterization tool of strongly correlated electron materials. Accurate calculation of RIXS spectra presents a significant challenge to theorists as it requires treating both highly local core-excited intermediate states as well as less localized and dispersing valence-excited final states. Furthermore, one must account for both quasiparticle and collective excitations, and any employed methodology should be extensible to strongly correlated materials. To calculate RIXS, and related core and valence level spectra, we solve the two-particle Bethe-Salpeter equation (BSE) based on a self-energy corrected density functional theory electronic structure. We discuss the suitability of this approach to a few systems of interest including strongly correlated 3d transition metal oxides (SrVO_3) and 5d TM-oxides (iridates).

RIXS can probe vibrational modes in addition to electronic excitations. Whereas other scattering techniques can only access phonon dispersion relations, RIXS is also sensitive to electron-phonon coupling strengths. We present a systematic, many-body theory approach for directly calculating the phonon RIXS spectrum and for quantifying the momentum dependent electron-phonon coupling strength. Numerical results are given for simple molecular systems and formal generalizations to periodic systems are presented.