

Abstract Submitted
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Vibrational effects on SrTiO_3 by K edge X-ray absorption using first-principle methods SILVIA TINTE, Ceramics Division, NIST, Gaithersburg, MD 20899-8520, ERIC L. SHIRLEY, Optical Division, NIST, Gaithersburg, MD 20899-8441 — Using the Bethe-Salpeter-equation methodology has recently become possible to calculate core and valence excited electronic states and spectra, which are usually computed in the ground-state atomic positions. However, vibrational effects can shift and broaden the spectrum through coupling atomic displacements to electron states and electronic excitations. In this work, we analyze the phonon effects on the Ti 3d states in cubic SrTiO_3 by Ti K edge X-ray absorption fine structure using first-principle methods. LDA total energies and coupled electron-hole Bethe-Salpeter equation calculations are performed for different ionic configurations following relevant normal modes of SrTiO_3 . As result, we obtain gradients of the excited-state energy and electron-phonon coupling coefficients. Our final goal is to include the Franck-Condon effect on the broadening of the calculated spectra.

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