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Numerical quantification of the vibronic broadening of the $SrTiO_3$ Ti L-edge spectrum KEITH GILMORE, ERIC SHIRLEY, National Institute of Standards and Technology — Calculations of x-ray absorption spectra are typically limited to obtaining the positions and intensities of spectral features, while simply adding broadening artificially to match experimental results. However, spectral widths hold valuable information on the coupling of the notional excited electronic state with the environment. The $2p^5 3d^1$ excited state of the Ti^{4+} ion in $SrTiO_3$ experiences Jahn-Teller coupling to e_g distortions of the oxygen cage. Such coupling broadens the electronic transition by involving a variable number of e_g phonons. We quantify this broadening effect by solving a model Hamiltonian, taking parameters for the Hamiltonian from first-principles calculations. Comparison of numerical and experimental results indicates that this vibronic coupling accounts for the majority of the broadening observed for the L_3-edge, but only a minority of the L_2-edge spectral width.

Keith Gilmore
National Institute of Standards and Technology

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