Abstract Submitted
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Finite temperature effects on the X-ray absorption spectra of energy related materials TOD PASCAL, DAVID PRENDERGAST, Lawrence Berkeley National Lab — We elucidate the role of room-temperature-induced instantaneous structural distortions in the Li K-edge X-ray absorption spectra (XAS) of crystalline LiF, Li_2SO_4, Li_2O, Li_3N and Li_2CO_3 using high resolution X-ray Raman spectroscopy (XRS) measurements and first-principles density functional theory calculations within the eXcited electron and Core Hole (XCH) approach. Based on thermodynamic sampling via *ab-initio* molecular dynamics (MD) simulations, we find calculated XAS in much better agreement with experiment than those computed using the rigid crystal structure alone. We show that local instantaneous distortion of the atomic lattice perturbs the symmetry of the Li 1s core-excited-state electronic structure, broadening spectral line-shapes and, in some cases, producing additional spectral features. This work was conducted within the Batteries for Advanced Transportation Technologies (BATT) Program, supported by the U.S. Department of Energy Vehicle Technologies Program under Contract No. DE-AC02-05CH11231.

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