Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Temperature dependence of Ti 1s near-edge spectra in Ti-based perovskites: theory and experiment ERIC SHIRLEY, ERIC COCKAYNE, BRUCE RAVEL, JOSEPH WOICIK, NIST — Ti 1s near-edge spectra (around 4970 eV) in $SrTiO_3$ and $PbTiO_3$ reveal electric-dipole and quadrupole transitions to Ti 3d, 4p and mixed 3d-4p states. Crystal field-split pre-edge features attributed to 1s→3d transitions are small compared to the main edge jump at the onset of the Ti 4s/4p continuum. Pre-edge and subsequent near-edge features are predicted to be weaker than what is observed, unless one accounts for ferroelectric polarization in $PbTiO_3$ and thermal motion in both compounds. Using density-functional theory molecular dynamics simulations at various temperatures (including sampling two phases of $PbTiO_3$), we capture the statistically averaged root-mean-square deviations of Ti^{4+} ions from the centers of their oxygen cages. By sampling appropriate snapshots of atomic configurations and averaging Ti 1s absorption spectra computed within a Bethe-Salpeter Equation framework, we obtain absorption spectra that agree well with experiment [R.V. Vedrinskii et al., J. Phys. IV France 7, C2-107 (1997), J.C. Woicik et al., Phys. Rev. B 75, 140103(R) (2007)], including details related to ferroelectric polarization, phase transitions, and fluctuations of atomic coordinates.

Eric Shirley
NIST

Date submitted: 10 Nov 2016 Electronic form version 1.4