

Abstract Submitted
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Correlations between tetragonality, polarization, and ionic displacement in lead titanate-derived ferroelectric perovskite solid solutions¹
ANDREW RAPPE, TINGTING QI, ILYA GRINBERG, University of Pennsylvania — We use first-principles density functional theory calculations to investigate the dependence of tetragonality on local structure in a variety of ferroelectric solid solutions. We demonstrate that tetragonality is strongly coupled to the *B*-cation displacement and weakly coupled to the *A*-cation displacement. Examination of various $\text{Bi}M^{3+}\text{O}_3$ additives to PbTiO_3 for different M^{3+} ionic sizes reveals that substitution of either small *B*-cations or low doping of large *B*-cations gives rise to large spontaneous polarization and tetragonality. Understanding how the phase transition temperature (T_c) and tetragonality are affected by Pb- and Bi-based perovskite additives provides a rational path for designing new high-temperature piezoelectric materials.

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