# Correlations between tetragonality, polarization, and ionic displacement in $PbTiO_3$-derived ferroelectric perovskite solid solutions

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## Abstract

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 $BiM^{3+}O_3$ 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.