Polarization enhancement in two- and three-component ferroelectric superlattices

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Composition-dependent structural and polar properties of epitaxial short-period $CaTiO_3/SrTiO_3/BaTiO_3$ superlattices grown on a $SrTiO_3$ substrate are investigated with first-principles density-functional-theory computational techniques. We find polarization enhancement with respect to bulk tetragonal $BaTiO_3$ in two- and three-component superlattices with high $CaTiO_3$ and $BaTiO_3$ concentration. The degree of the enhancement as well as polarization asymmetry due to inversion symmetry breaking in three-component superlattices can be controlled by varying the thicknesses and arrangement of the component layers, resulting in more efficient and flexibly tuned lead-free nano-electro-mechanical devices.