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First-principles modeling of piezoelectric response of perovskite superlattices: the case of $BaTiO_3/CaTiO_3$ QIBIN ZHOU, KARIN RABE, Rutgers University — In multicomponent ABO_3 superlattices, instabilities belonging to individual bulk constituents strongly interact with each other through the interfaces. Such interactions in superlattices lead to rich behavior beyond that of simple perovskites, and in particular can lead to enhanced piezoelectric response.* In this work, we studied short-period $BaTiO_3/CaTiO_3$ superlattices with varying layer thicknesses and overall composition. Our first-principles calculations reveal a phase transition between ferroelectric and dielectric phases at a $BaTiO_3$ fraction close to 50% and enhanced piezoelectricity in the ferroelectric phase. A first-principles-based model, extending a previous analysis for $PbTiO_3/BaTiO_3$ superlattices, is constructed to predict the phase transition, the polarization and tetragonality, and the enhanced piezoelectricity. The further extension of this modeling approach to a wider range of perovskite superlattices will be discussed.

*V. R. Cooper and K. M. Rabe, Phys. Rev. B 79, 180101 (2009).

Qibin Zhou
Rutgers Univ

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