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First-principles study of symmetry lowering in relaxed $BaTiO_3/SrTiO_3$ superlattices KAREN JOHNSTON, Rutgers University, XIANGYANG HUANG, University of Minnesota, JEFFREY B. NEATON, University of California Berkeley, KARIN M. RABE, Rutgers University — The crystal structure and local spontaneous polarization of $(BaTiO_3)_m/(SrTiO_3)_n$ superlattices is calculated using a first-principles density functional theory method. The in-plane lattice constant is 1% larger than the $SrTiO_3$ substrate to imitate the relaxed superlattice structure and the symmetry is lowered to monoclinic space group Cm which allows polarization to develop along the [110] and [001] directions. The polarization component in the [110] direction is found to develop only in the $SrTiO_3$ layers and falls to zero in the $BaTiO_3$ layers, whereas the polarization in the [001] direction is approximately uniform throughout the superlattice. These findings are consistent with recent experimental data and first-principles results for epitaxially strained BT and ST.

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