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First-principles study of piezoelectric response in $PbTiO_3/SrTiO_3$ 1 x 1 superlattice[1] YANPENG YAO, HUAXIANG FU, Department of Physics, University of Arkansas — Artificial superlattices composed of two materials of similar structure but distinct properties are a promising group of new materials to achieve modified properties. For ferroelectric materials, it is well known that strain effects due to lattice mismatch can considerably alter the properties of ferroelectric thin films. Here we perform first-principles density functional calculations to study the structure and polarization response of $PbTiO_3/SrTiO_3$ (PT/ST) 1x1 superlattice to varied inplane strain. The superlattice is chosen to be grown along the [001] crystallographic direction, and is assumed to be tetragonal. For a given inplane strain, the out-of-plane lattice constant and atomic positions are relaxed. Similar calculations on PT, ST single materials are also performed for comparison. We find that by increasing strain, the superlattice has combined features as those of PT and ST single materials. Being unpolar without strain, the superlattice becomes ferroelectric at a critical inplane lattice constant larger than that of ST. The PT/ST 1x1 superlattice is shown to have a much larger piezoelectric response than PT, a property similar to ST. But, compared to ST, the large piezoelectric response in PT/ST is easier to realize, since a smaller inplane strain is required.

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