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**Interplay of couplings between antiferrodistortive, ferroelectric, and strain degrees of freedom in monodomain $PbTiO_3/SrTiO_3$ superlattices**[1] PABLO AGUADO-PUENTE, PABLO GARCIA-FERNANDEZ, JAVIER JUNQUERA, DCITIMAC, Universidad de Cantabria, Avda. de los Castros s/n, 39005 Santander, Spain — We report first-principles calculations, within the density functional theory, on the coupling between epitaxial strain, polarization, and oxygen octahedra rotations in monodomain $(PbTiO_3)_n/(SrTiO_3)_n$ superlattices. We show how the interplay between (i) the epitaxial strain and (ii) the electrostatic conditions at the interfaces can be used to control the orientation of the main axis of the system – defined by the direction of the polarization or the rotation axis of the oxygen octahedra. The electrostatic constrains at the interface facilitate the rotation of the polarization and, as a consequence, we predict large piezoelectric responses at epitaxial strains smaller than those that would be required considering only strain effects. In addition, ferroelectric (FE) and antiferrodistortive (AFD) modes are strongly coupled, with different rotation angles in the $TiO_6$ octahedra as a function of the polarization direction. The magnitude of the rotations cannot be explained by the usual steric arguments alone, and a covalent model is proposed to account for the large polarization-tilting coupling. The energy gain due to the FE-AFD coupling decreases with the periodicity of the superlattice, becoming negligible for $n \geq 3$.

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