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Strain-coupled octahedral tilts and local polar displacements in superlattices[1] JOSEPH SCHICK, Villanova Univ, LAI JIANG, DIOMEDES SALDANA-GRECO, ANDREW RAPPE, Univ of Pennsylvania — The ability to manipulate octahedral tilts and (anti-)ferroelectric polar displacements in perovksites is a path that opens the possibility of creating new materials with desirable optical, electric, and magnetic properties. We present a density functional investigation of the ability to control tilts and displacements in various short-period superlattices composed of absent-A-site perovskites WO_3 and ReO_3. We demonstrate that rotations and displacements of the B-cations in WO_3 are altered when layered with ReO_3. We also determine the thermodynamic stability of the superlattices, showing that ReO_3 fraction $> 50\%$ and with at least three ReO_3 layers are stable.

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