Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

The $CdTiO_3/BaTiO_3$ Superlattice Interface from First Principles

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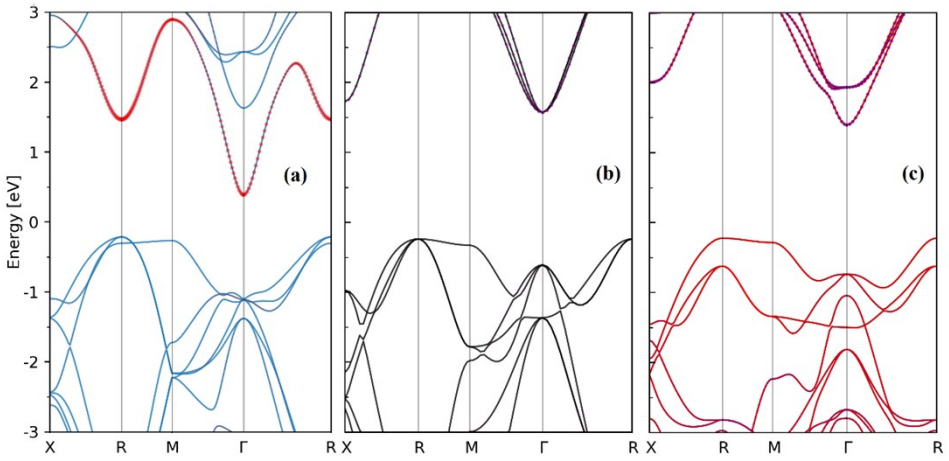

Figure S1. Orbital-projected band structures for conduction bands of bulk-phase (a) $CdTiO_3$ with in-plane lattice constant of $BaTiO_3$, (b) cubic $SrTiO_3$ and (c) tetragonal $BaTiO_3$. The red dots are for Cd-5s states and the purple dots are for Ti-3d states.

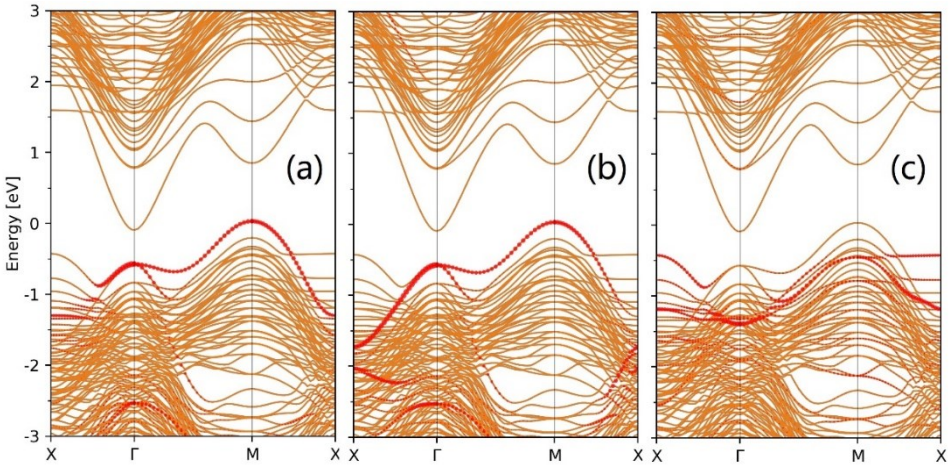

Figure S2. Orbital-projected band structures for the O 2p states of the p-type conductivities in $(CdTiO_3)_4/(BaTiO_3)_8$ superlattice. The red circles in (a), (b) and (c) are for p_x, p_y and p_z orbitals respectively.

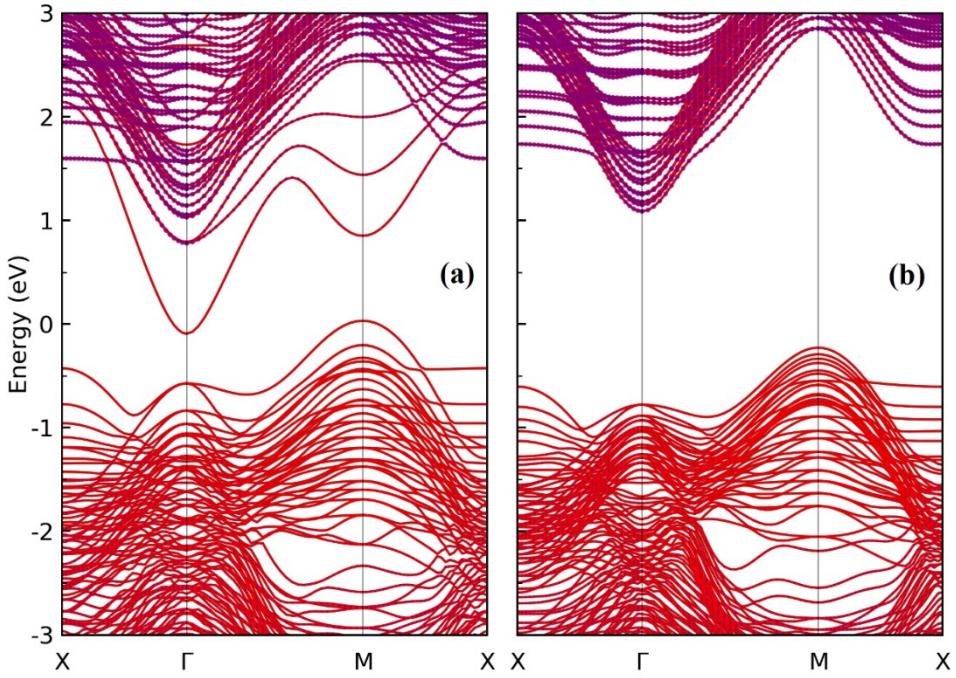

Figure S3. Orbital-projected band structures for Ti 3d states of (a) $(CdTiO_3)_4/(BaTiO_3)_8$ and (b) $(SrTiO_3)_4/(BaTiO_3)_8$ superlattices.

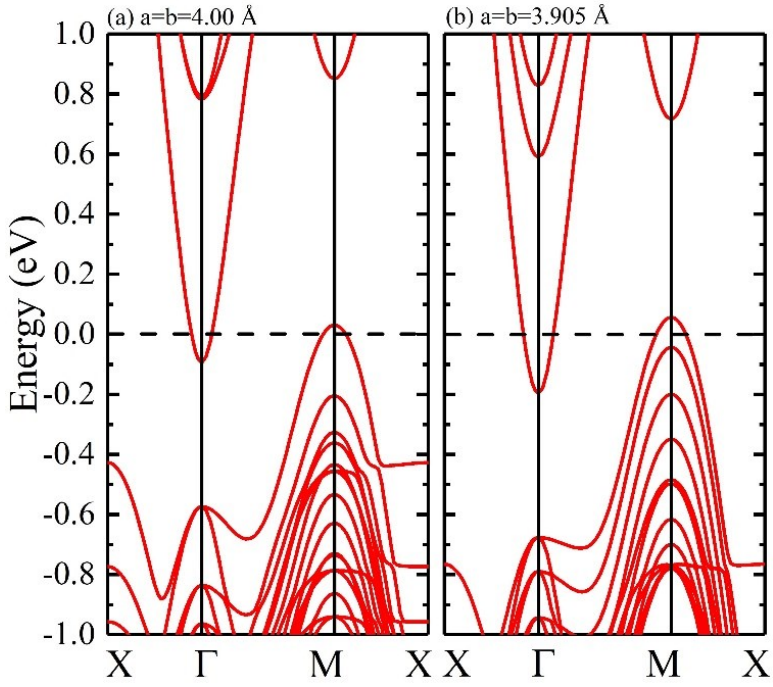

Figure S4. The calculated band structures for the $(CdTiO_3)_4/(BaTiO_3)_8$ superlattice of (a) a=b=4 Å and (b) a=b=3.905Å.

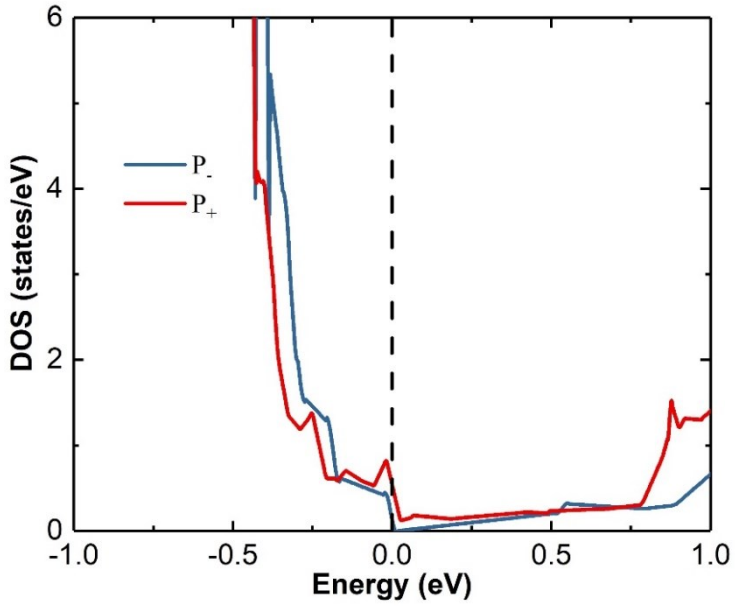

Figure S5. The calculated total density of states (DOS) for P_+ and P_- of the $(CdTiO_3)_4/(BaTiO_3)_8$ superlattice.

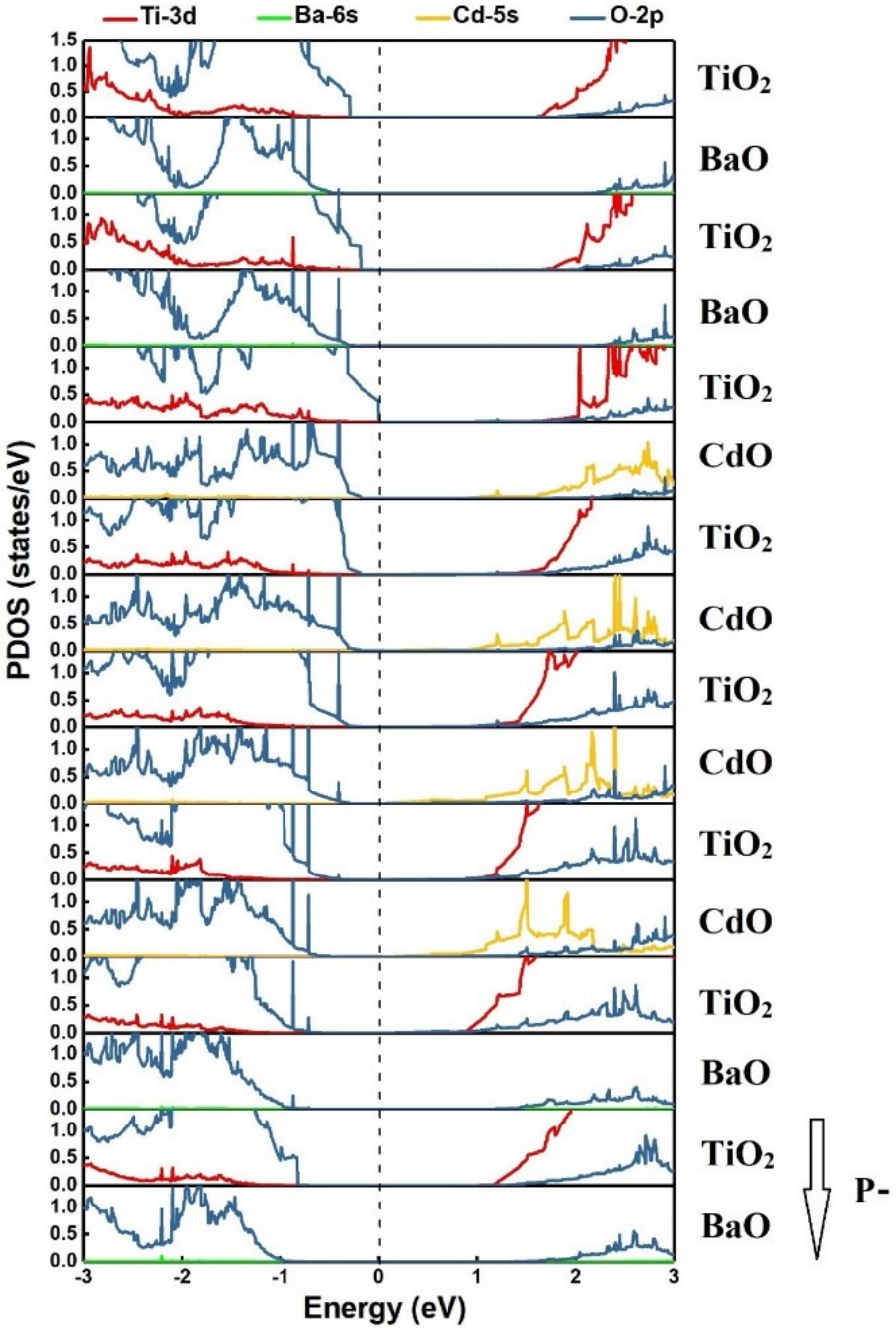

Figure S6. The calculated layer-resolved partial DOS for the $(CdTiO_3)_4/(BaTiO_3)_8$ superlattice along P- direction in the range from -3.0 eV to 3.0 eV on each BaO, CdO and TiO_2 layer.

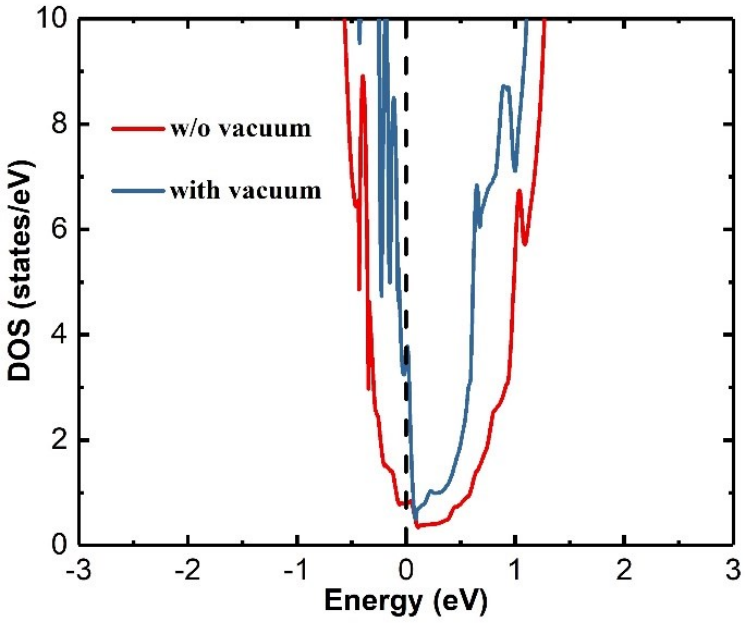

Figure S7. The calculated total density of states (DOS) for the supercell model (without vacuum) and thin film model (with vacuum) of the $(CdTiO_3)_8/(BaTiO_3)_6$ heterostructure.

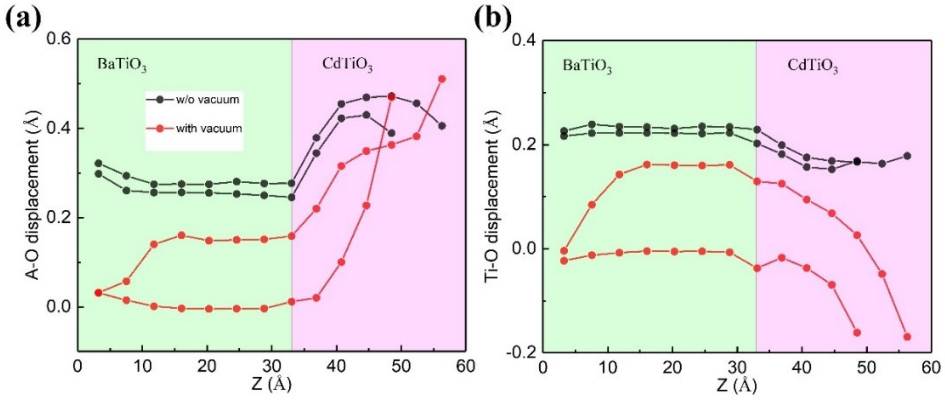

Figure S8. Structural distortions in the $(CdTiO_3)_n/(BaTiO_3)_8$ heterostructure (n=4 and 6) with the change in the number of $CdTiO_3$ layers along c-axis for (a) A-site cation (Cd in $CdTiO_3$ and Ba in $BaTiO_3$) displacements and (b) B-site cation (Ti in $CdTiO_3$ and $BaTiO_3$) displacements along the c-axis with respect to the oxygen in the plane. The black/red line is the supercell/thin film model without/with vacuum, respectively.