Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Design Two-Dimensional Electron Gas via Polarization Discontinuity from Large-Scale First-Principles Calculations

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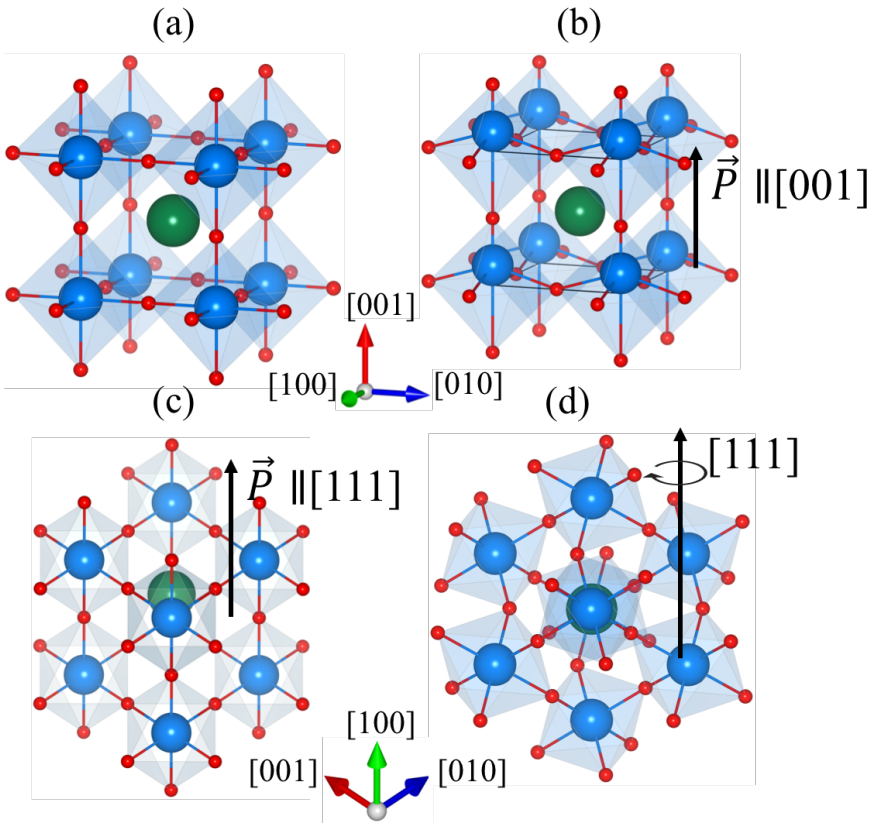

Figure S1. Scheme of perovskite oxide ABO_3 structures: (a) cubic, (b) tetragonal, (c) rhombohedral, and (d) structure with oxygen octahedral rotates along the [111] direction.

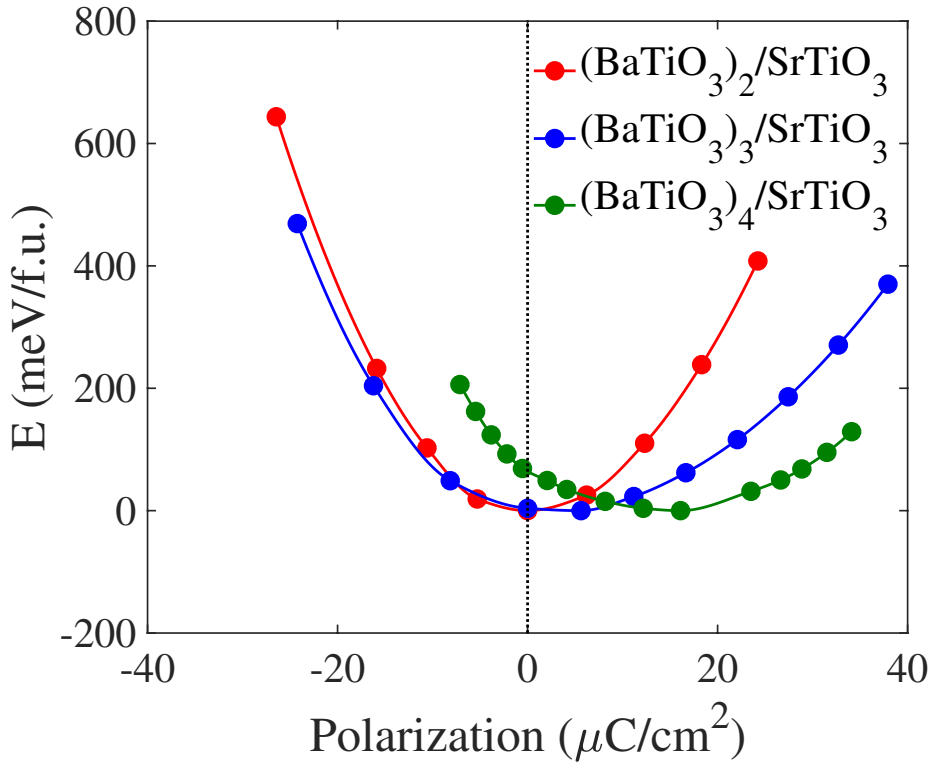

Figure S2. Calculated total energy per unit cell of the film as a function of the average polarization for $BaTiO_3/SrTiO_3$ heterostructure (HS) models with different film thickness. The reference energy (zero) is taken from the lowest energy of each system.

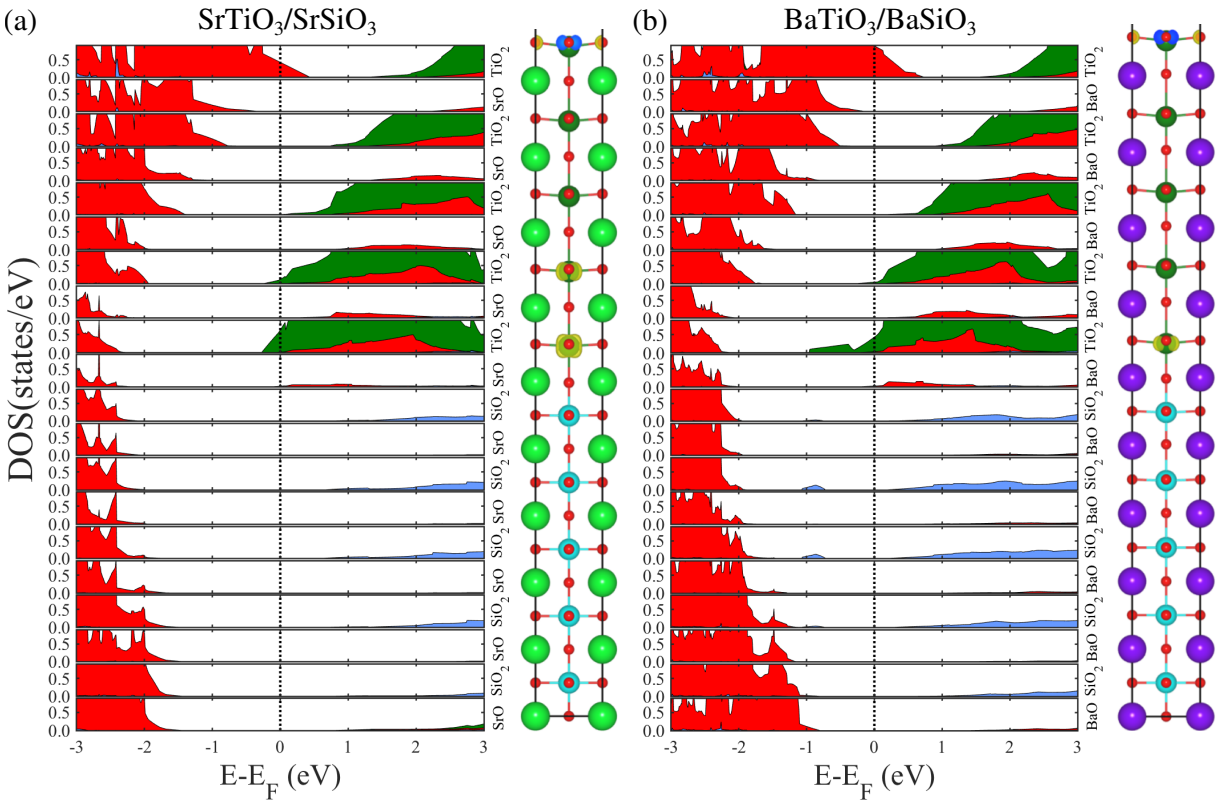

Figure S3. Calculated layer-resolved partial DOS for (a) $SrTiO_3/SrSiO_3$ and (b) $BaTiO_3/BaSiO_3$, along with their charge density plots projected on the bands forming the metallic states. The vertical dash line at zero-point energy shows the Fermi level. The solid blue, red, and green color indicates *s*, *p*, and *d* orbital, respectively.

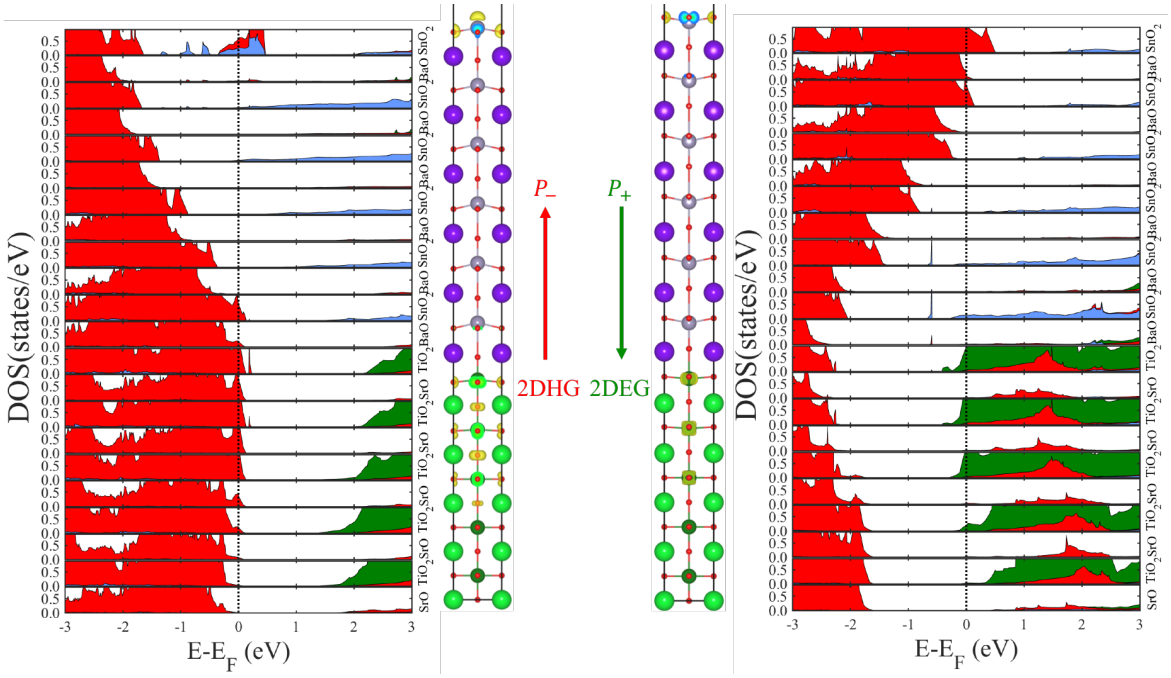

Figure S4. Calculated layer-resolved partial DOS for P_+ and P_- states in $BaSnO_3/SrTiO_3$ HS, along with their charge density plots projected on the bands forming the metallic states.

Table S1. Calculated electron effective mass m^* (in unit of free electron mass) along the M-Γ and Γ-X path for $BaTiO_3/SrTiO_3$, $CaZrO_3/YbZrO_3$, $CaZrO_3/CaHfO_3$, $CaSnO_3/BaSiO_3$, $BaSiO_3/CaGeO_3$, and $CaZrO_3/SrSnO_3$ HS models.

Systems	m^*/m_e		
	M-Γ	Γ-X	Average
$BaTiO_3/SrTiO_3$	0.56	0.46	0.51
$CaZrO_3/YbZrO_3$	0.40	0.38	0.39
$CaZrO_3/CaHfO_3$	0.51	0.40	0.46
$CaSnO_3/BaSiO_3$	0.34	0.31	0.33
$BaSiO_3/CaGeO_3$	0.30	0.24	0.27
$CaZrO_3/SrSnO_3$	0.34	0.28	0.31