Electronic Supplementary Material (ESI) for RSC Advances.
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Supplementary Information

The origins of charge separation in anisotropic facets photocatalyst investigated through first-principles calculations

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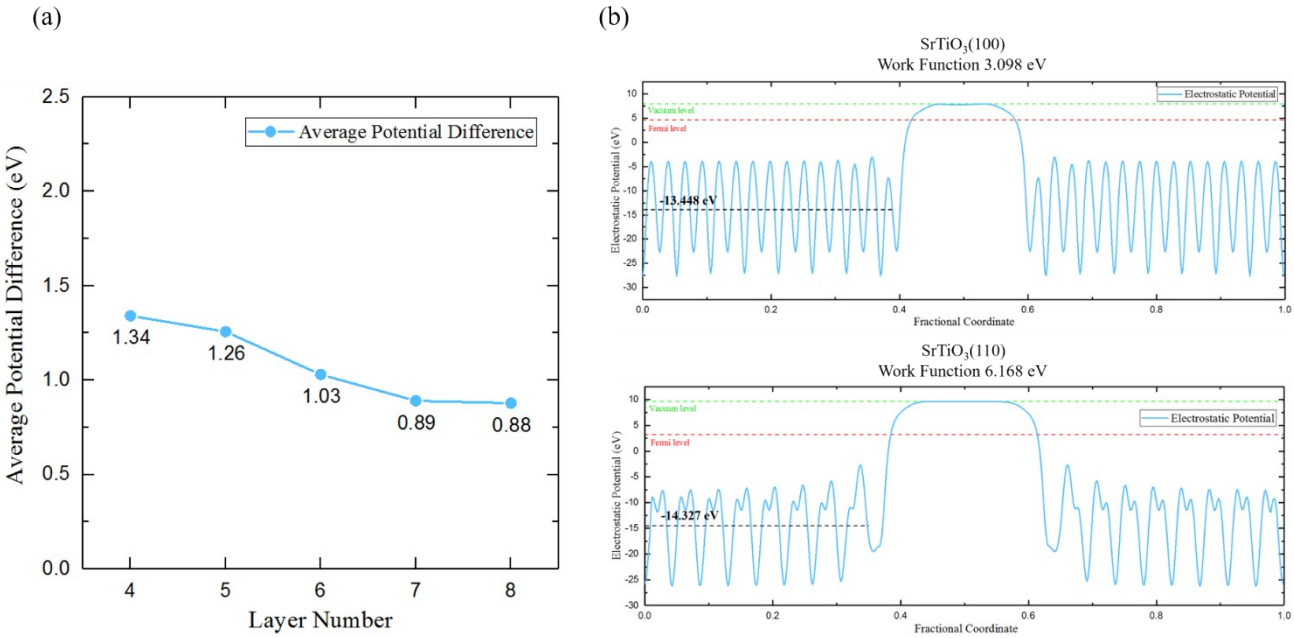

Fig. S1. (a) Convergence of surface layers tested for four to eight layers of (100) and (110) planes. (b) Eight layers was found to be sufficient for convergence in both (100) and (110) models. The average potential difference is calculated for the macroscopic average electrostatic potential (MAEP) on the side of the vacuum region for (100) and (110) planes. For instance, the MAEP of the side region for (100) and (110) are -13.448 eV and -14.327 eV, respectively, and the average potential difference is therefore calculated as $-13.448-(-14.327)=0.879$ eV.

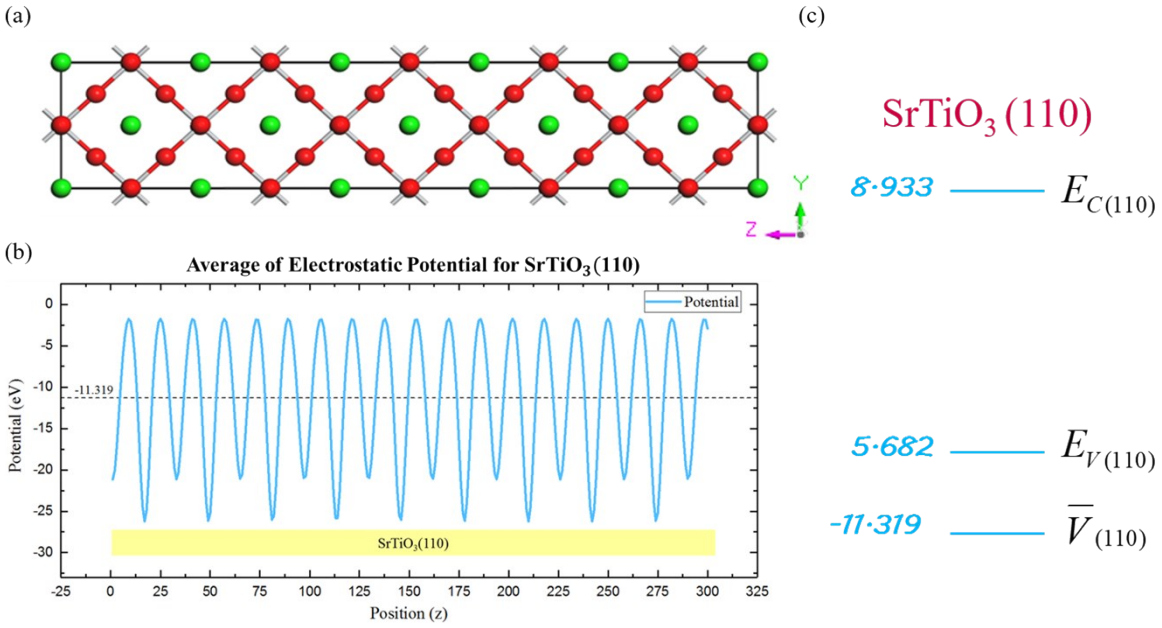

Fig. S2. (a) The superlattice, (b) average electrostatic potential, and (c) band diagram of (110) plane. The MAEP, VBM, and CBM of (110) are -11.319 eV, 5.682 eV, and 8.933 eV, respectively.

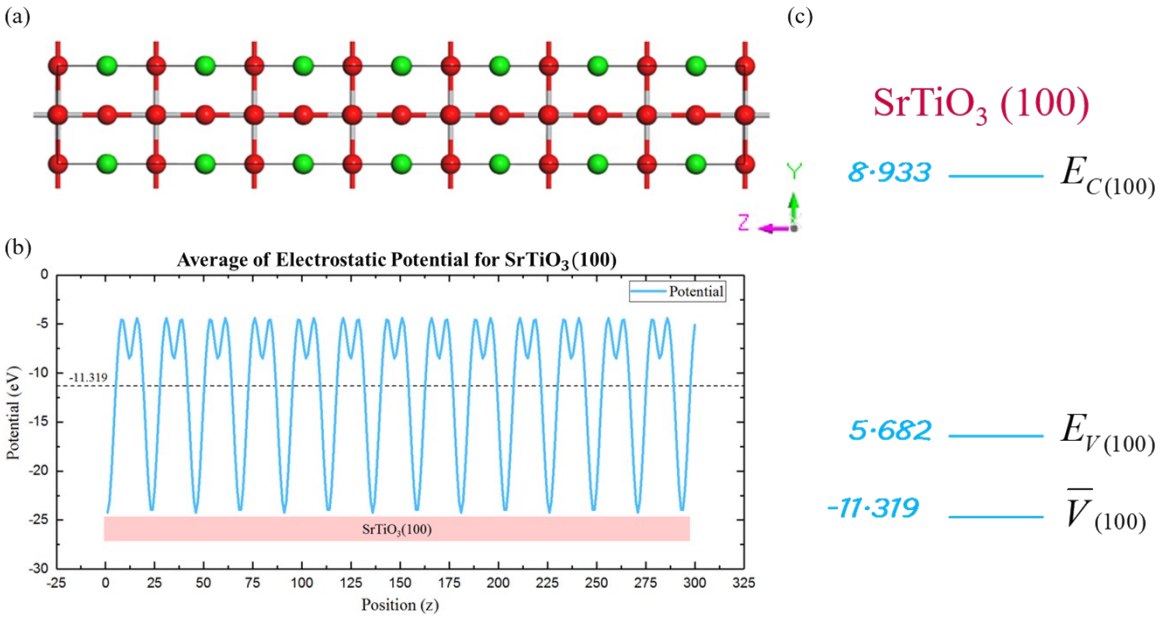

Fig. S3. (a) The superlattice, (b) average electrostatic potential, and (c) band diagram of (100) plane. The MAEP, VBM, and CBM of (100) are -11.319 eV, 5.682 eV, and 8.933 eV, respectively.

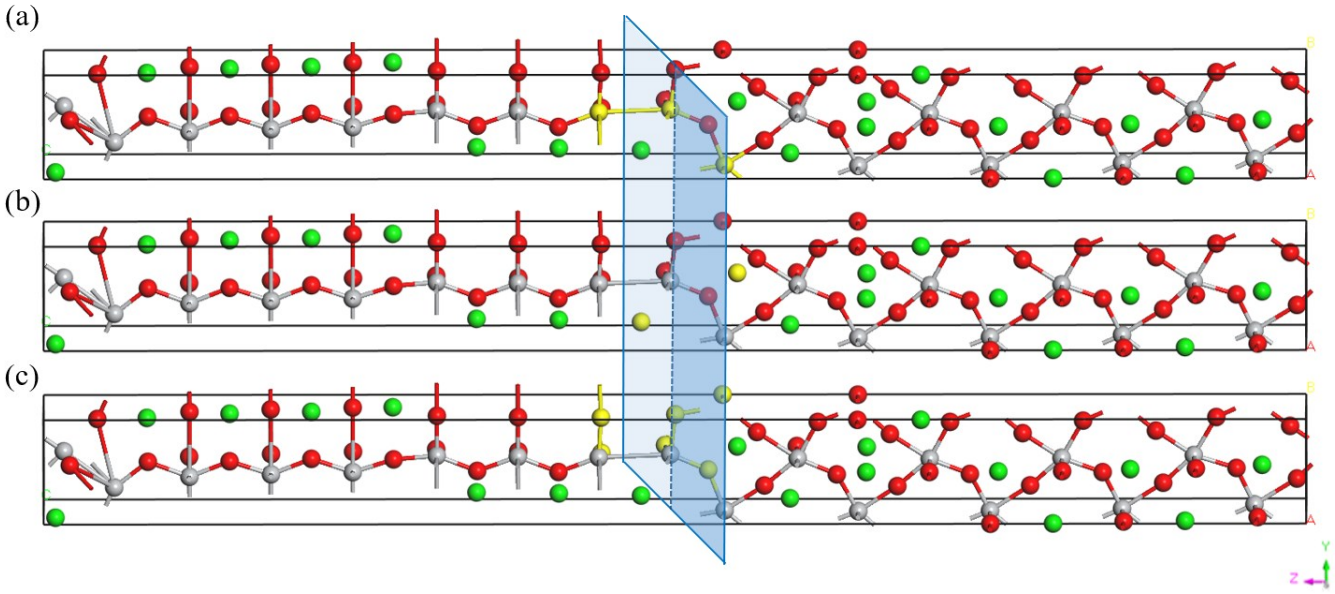

Fig. S4. The selected (a)Ti, (b)Sr, and (c) O atoms locate near the junction for PDOS comparison with bulk electronic structure. The blue plane is the interface between (100) and (110), with Ti atom located directly on the plane.

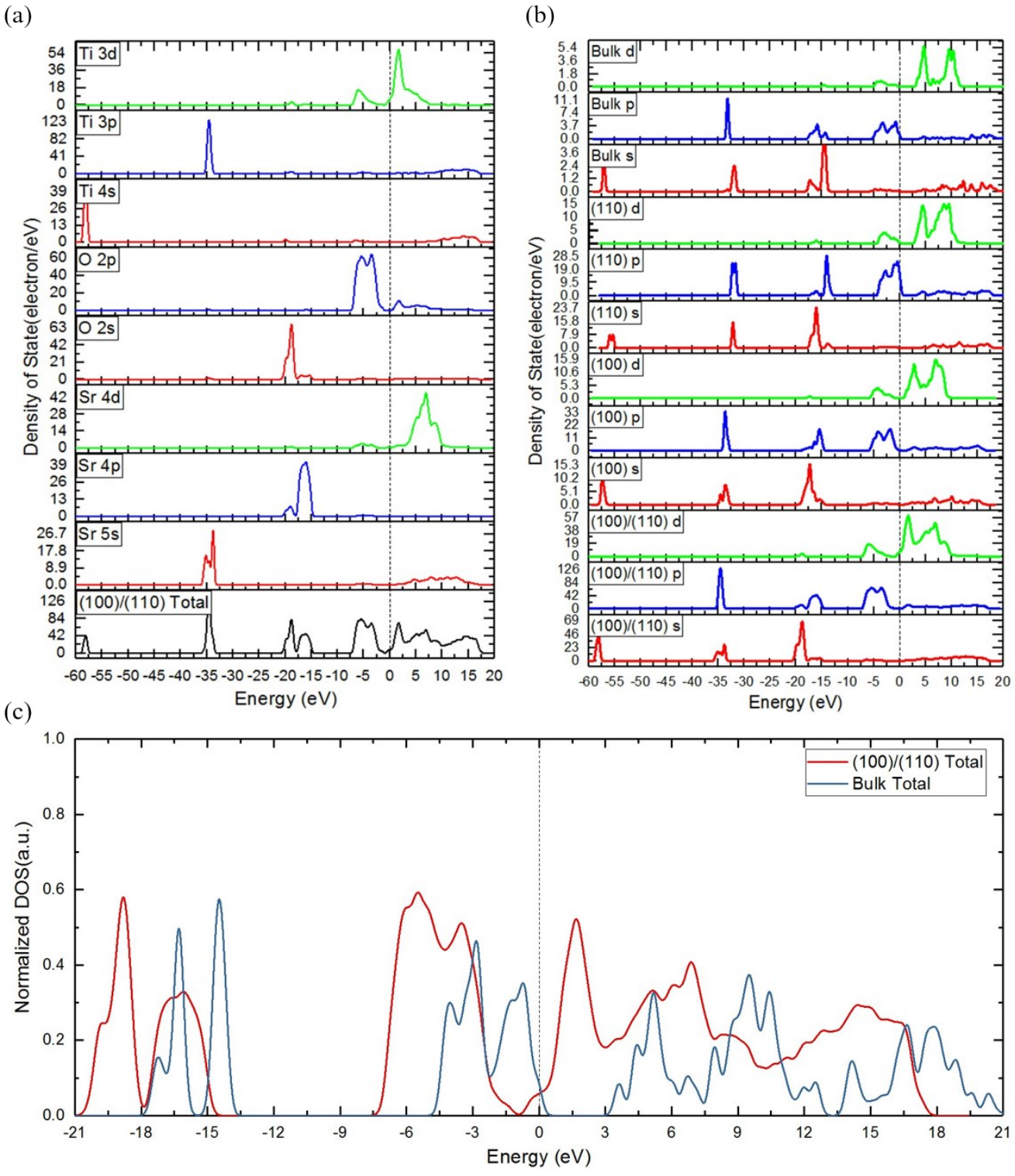

Fig. S5. (a) The PDOS of (110)/(100) facet junction, (b) PDOS of *s*, *p* and *d* atomic orbitals in bulk, plane, and facet junction, and (c) normalized DOS of bulk and facet junction. The Fermi level is set to the zero point energy.