Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Interfacial Band Offset Engineering with Barium-doping Towards Enhanced Performance of all Inorganic $CsPbI_2Br$ Perovskite Solar Cells

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Figure S1. (a and b) Optimized structure for $CsPbI_2Br(010)$ and $Ba:CsPbI_2Br(010)$ surfaces.

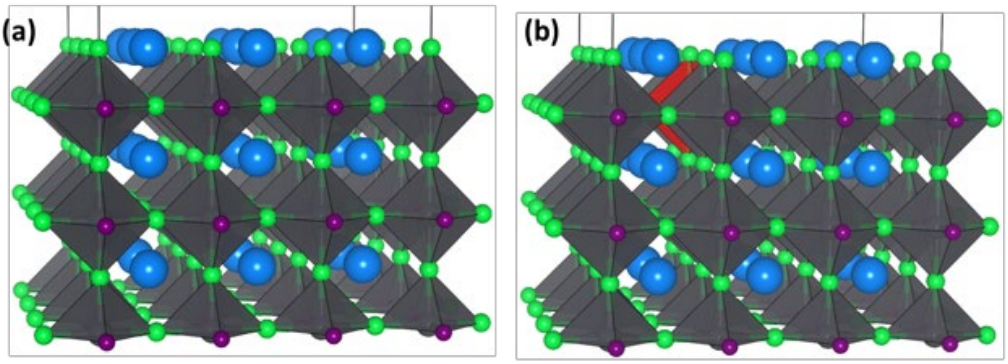

Figure S2. (a) Electronic band structures of bulk anatase TiO_2 for Ti-d (blue) and O-p (red) orbitals. Inset: Crystal structure of TiO_2. (b) Anatate TiO_2 (ETL) modelled in the tetragonal structure predicting the lattice parameters at a=b=3.803 Å, c=9.517 Å, in good agreement with the experimental values.