

Supporting information for
Interface Engineering using Perovskite Derivative-Phase for Efficient
and Stable CsPbBr₃-Solar Cells

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Experimental Section

Inorganic perovskite films: The inorganic perovskite films were prepared by the vapor deposition approach. Firstly, the CsBr, PbBr₂ precursors and substrates were placed in the vacuum system, and pumped to the vacuum degree of $\sim 10^{-4}$ Pa. Secondly, a CsBr film of thickness ~ 100 nm was formed on the substrates with an evaporation rate of ~ 0.4 Å/s in a lower vacuum system. Then the PbBr₂ film was coated upon the as-deposited CsBr film with an evaporation rate of ~ 1 Å/s with different thickness. The final inorganic perovskite films were obtained after a simple heating at 150 °C for 10min in the air.

Device Construction: The acetone, ethyl alcohol and deionized water were used as detergent solution to wash the FTO glasses by sonication, sequentially. Then the FTO substrates were dried in a circulation oven at 70 °C. The electronic transfer layer was formed by spin-coated the titanium isopropoxide precursor solution at a speed of 2000 rpm for 40s and annealed at 500 °C for 0.5 h in the furnace. After cooling to room temperature, the substrates were treated in 40 mM aqueous solution of TiCl₄ at 70 °C and heated at 500 °C for 0.5 h, respectively. Afterwards, the inorganic perovskite films

were deposited on the FTO/c-TiO₂ substrates via a vapor deposition approach. Hole transfer layer was formed upon the inorganic perovskite layer by spin-coated the Spiro-OMeTAD precursor solution at 3500 rpm, 30s. Finally, the 120 nm thickness silver electrode was formed on the top of the devices by thermal evaporation. The active area of all devices active is 0.09 cm².

Measurements: XRD patterns of as-synthesized film were identified using the X-ray powder diffraction (XRD) with a Cu K α radiation (scanning range: 10°~70°). The instrument to analyze the composition of inorganic perovskite film was X-ray photoelectron spectra (XPS, Thermo ESCALAB 250). The morphology of the samples was investigated in a field emission scanning electron microscopy (FE-SEM, Sigma Zeiss). The absorption and PL spectrum of inorganic perovskite film were performed using a UV-visible spectrophotometer (UV-2550) and a Hitachi F-4600 fluorescence spectrophotometer, respectively. Photocurrent density–voltage (J-V) measurements of perovskite solar cells were carried out on a Keithley 2636 system sourcemeter equipped with a Xenon Lamp Solar Simulator. The light intensity was ~100 mW cm⁻². All the measurements were performed at the room temperature with the relative humidity below 45%.

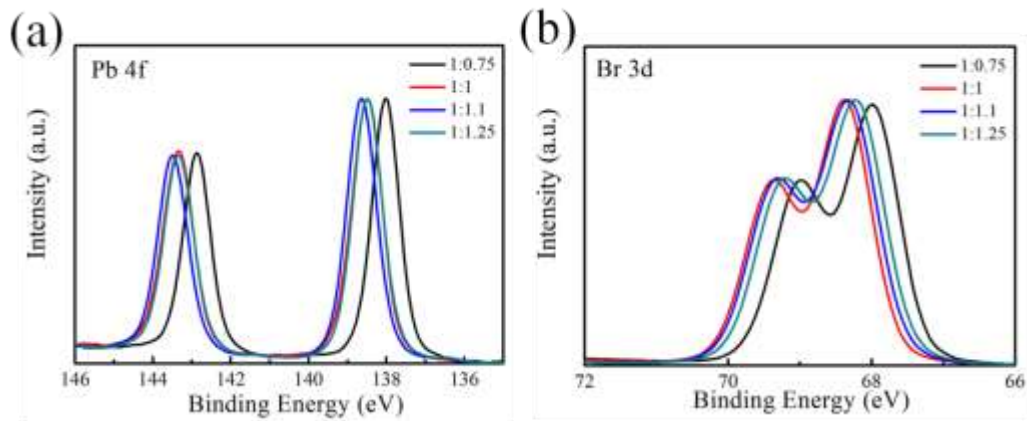


Fig. S1 XPS spectrum of the (a) Pb 4f and (b) Br 3d for inorganic perovskite film with various ratios.

Table S1 The ratio of Cs to Pb and Br deduced from XPS measurements of inorganic perovskite film with various ratios.

Ratio	1:0.75	1:1	1:1.1	1:1.25
Cs/Pb	1:0.57	1:0.93	1:2.42	1:3.37

Cs/Br	1:2.29	1:3.19	1:5.89	1:8.73
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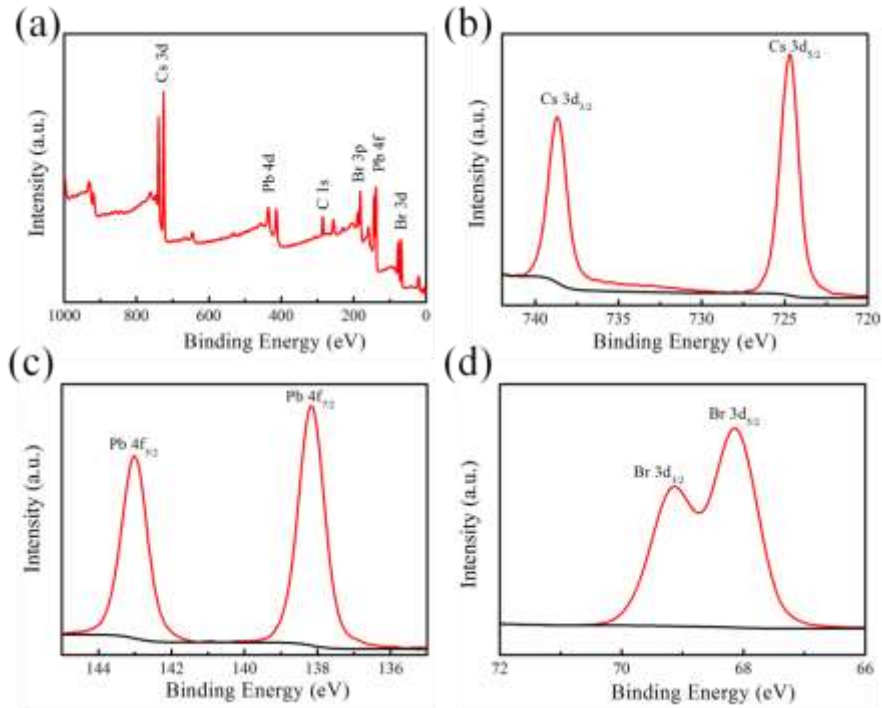


Fig. S2 XPS spectrum of the (a) Overall, (b) Cs 3d, (c) Pb 4f and d) Br 3d for derivative -phase inorganic perovskite film.

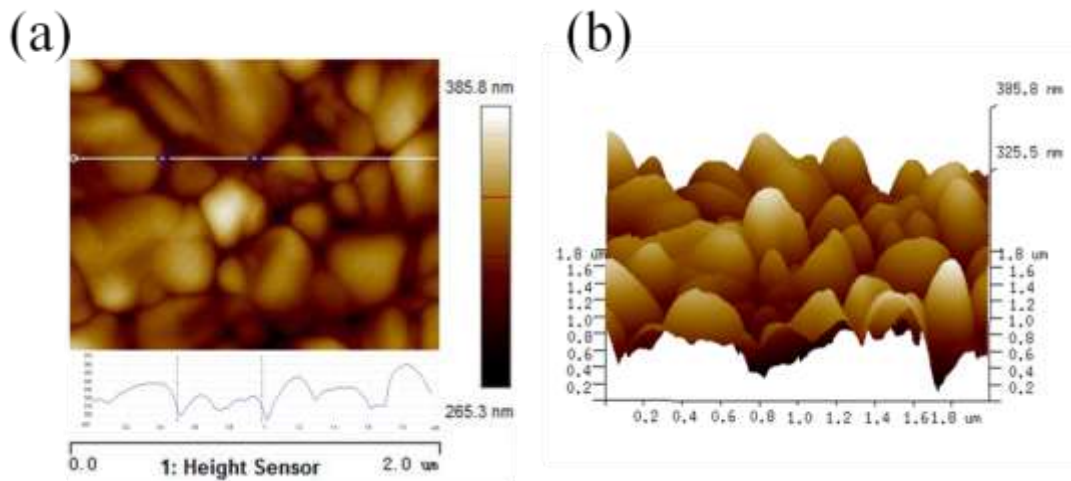


Fig. S3 (a) 2D and (b) 3D AFM characterizations of the inorganic perovskite film with the ratio of 1:1.1.

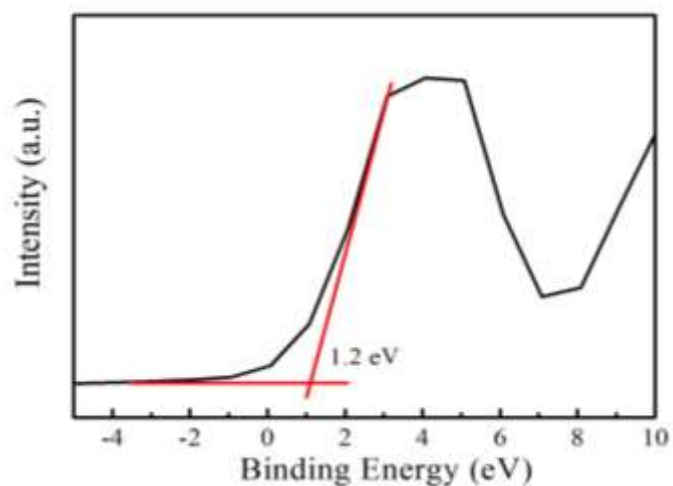


Fig. S4 Valence band XPS spectrum of derivative-phase ($\text{CsPBr}_3\text{-CsPb}_2\text{Br}_5$) inorganic perovskite film. The spectrometer work function of the XPS instrument applied in our work is near to -4.2 eV. And the valence band maximum (VBM) of $\text{CsPBr}_3\text{-CsPb}_2\text{Br}_5$ was determined by taking a linear extrapolation and was estimated to be -5.4 eV, as witnessed in Figure 3b. In addition, Figure 1b infers that the optical band gap of $\text{CsPBr}_3\text{-CsPb}_2\text{Br}_5$ is 2.4 eV. Therefore, the conduction band minimum (CBM) of $\text{CsPBr}_3\text{-CsPb}_2\text{Br}_5$ film was calculated to be -3.0 eV.