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Supporting Information

Crosslinked Thioctic Acid as Multifunctional Buried Interface Modifier for High Performance Inorganic Perovskite Solar Cells

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Experimental Section

Materials and Reagents:

Lead iodide (PbI_2, 99.9%), Lead bromide ($PbBr_2$, 99.9%), and Cesium iodide (CsI, 99.9%) were purchased from Xi'an Polymer Light Technology Corp. The polymer donor materials PM6 was bought from Organtec Ltd. The α-thioctic acid (TA, 99%), zinc acetate dihydrate (>98%) and Ethanolamine (99.5%) were purchased from Aladdin. N, N-dimethylformamide (DMF, 99.8%), dimethyl sulfoxide (DMSO, 99.8%, anhydrous), and chlorobenzene (CB, 99.8%) were got from Sigma-Aldrich. Molybdenum Trioxide (M_OO_3, 99.99%) was purchased from Alfa Aesar. All the available reagents were used as received without any further purification unless otherwise specified.

Device Fabrication:

The planar PSCs were fabricated using the device configuration of ITO/ETL/$CsPbI_2Br$/PM6/MoO_3/Ag. Patterned ITO substrates were sequentially ultrasonicated in detergent, deionized water, acetone, and isopropanol, and then were treated with O_2-plasma for 8 min. The ZnO precursor was prepared by dissolving 1 g zinc acetate dihydrate in 10 mL 2-Methoxyethanol and 275 μL Ethanolamine. Then the ZnO precursor was spin-coated on the substrate at 4000 rpm for 40 s, followed by heating at 150 ° C for 20 min. Subsequently, the TA modifier is deposited on the ZnO layer by spin-coating isopropanol solution containing TA molecules, followed by annealing treatment at 100 °C for 10 min. After that, the substrates were transferred to a glove box filled with N_2. The precursor solution of $CsPbI_2Br$ perovskite was prepared by dissolving 0.9 M CsI, 0.45 M PbI_2 and 0.45 M $PbBr_2$ in the DMF/DMSO (7:3) solvent with stirring at 60 °C overnight. And the filtered $CsPbI_2Br$ precursor solution was dropped on the ITO/ETL substrates via a

two-step proceture at 1200 rpm for 40 s and thermal annealed at 40 °C for 60 s and 180 °C for 5 min. When the films were cooled to room temperature, PM6 (6 mg in 1 mL of chlorbenzene (CB) solution without any dopants) was spin-coated on the perovskite films at 1500 rpm for 30 s and then annealed at 100 °C for 5 min to form the hole-transporting layer. Finally, a 8 nm MoO_3 and 100 nm Ag were thermally evaporated under high vacuum ($< 2 \times 10^{-4}$ Pa), respectively. The effective device area was defined to be ≈0.09 cm^2 controlled with a shadow mask.

Characterizations and Measurements:

UV-vis absorption spectra were recorded with a GS54T UV-vis-NIR absorption spectrophotometer. The steady-state fluorescence (PL) and time resolved photoluminescence (TRPL) spectra of the films were collected by Fluorolog-Horiba with excitation wavelength of 400 nm and Delta Flex Fluorescence Lifetime System (Horiba Scientific Com., Japan), respectively. XRD patterns were collected at Bruker AXS D8 Advanced (Germany) equipped with Cu K_α radiation ((λ= 0.154 nm). The morphology of $CsPbI_2Br$ films images were obtained with the field emission scanning electron microscope (Hitachi, S-4800). And the tapping-mode atomic force microscopy (AFM) images were conducted by using a scanning probe microscope (Dimension 3100 V, Veeco). The chemical states of the film surface were explored by X-ray photoelectron spectroscopy (XPS, Kratos AXIS ULTRA DALD) tests. The *J-V* characteristics were measured with a Keithley 2400 source meter by using a So13A solar simulator (Newport Inc.) with an AM 1.5G irradiation intensity (100 mW cm^{-2}). The external quantum efficiency (EQE) measurements were using a Newport EQE system in ambient atmosphere. The transient photocurrent (TPC) decay and transient photovoltage (TPV) decay were conducted on

electrochemical workstation (Zahner, Germany) with an 80 mW/cm^2 white light illuminated.

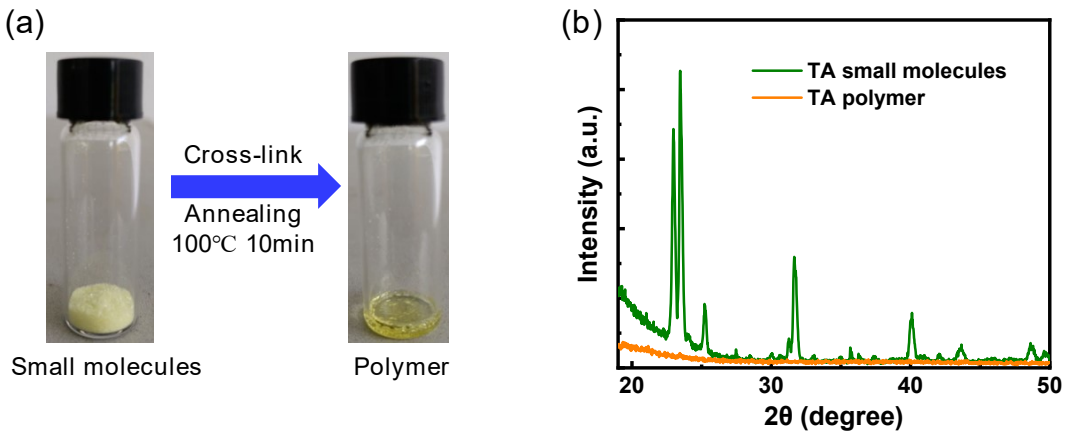

Fig. S1 (a) Photographs of TA molecules before and after annealing treatment. (b) XRD patterns of TA molecules before and after annealing treatment.

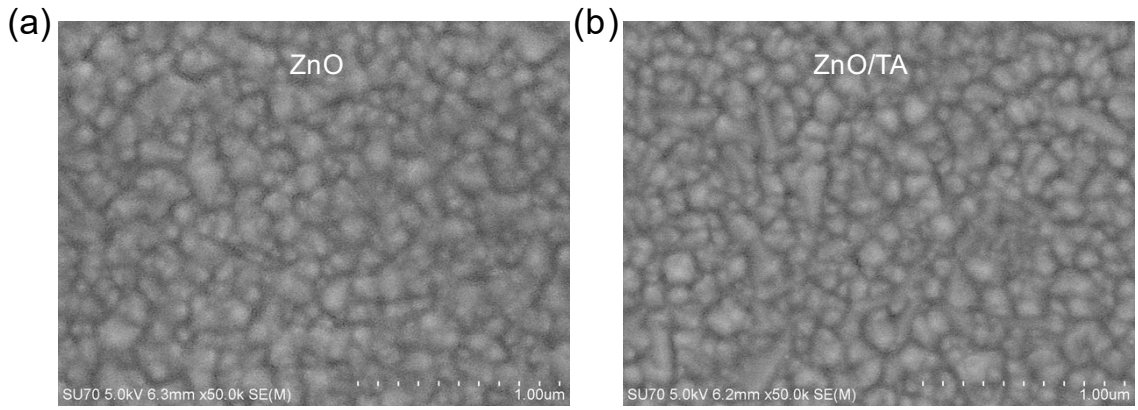

Fig. S2 Top-view SEM images of the (a) bare ZnO, and ZnO/TA films.

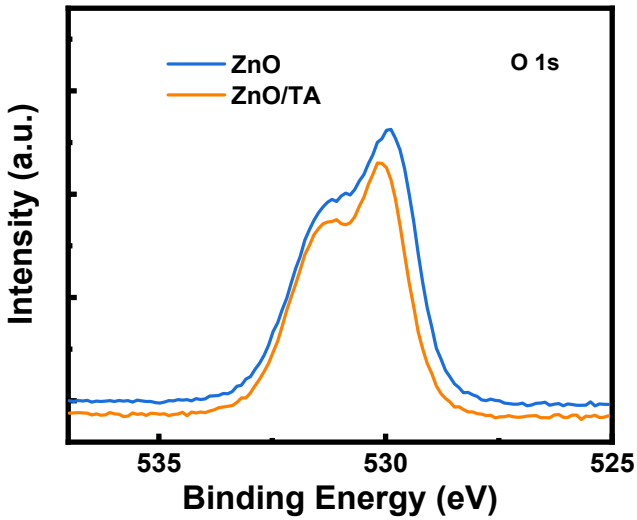

Fig. S3 The XPS spectra of O 1s core levels of bare ZnO, and ZnO/TA films.

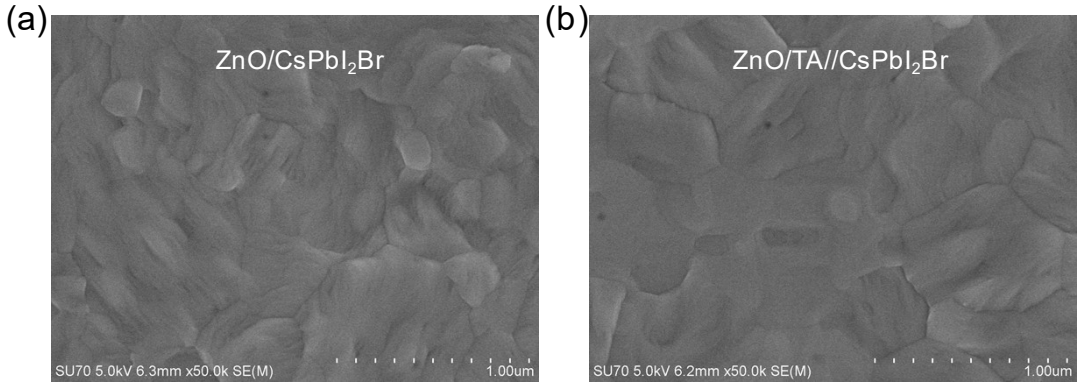

Fig. S4 Magnified SEM images of the $CsPbI_2Br$ film on (c) ZnO, and (d) ZnO/TA ETLs.

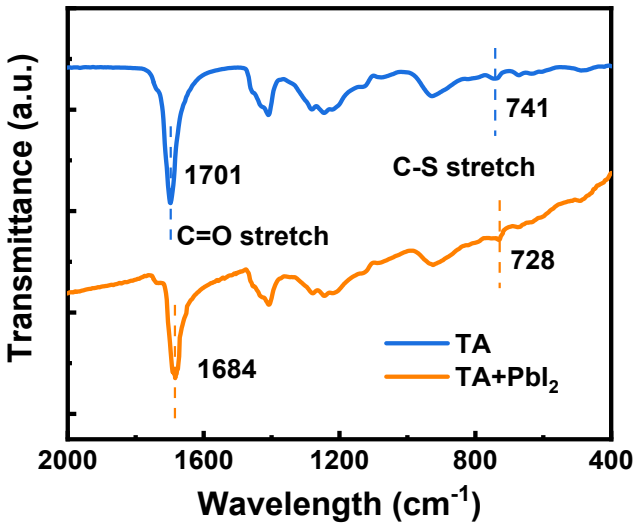

Fig. S5 FTIR spectra of TA and TA+PbI_2 complex.

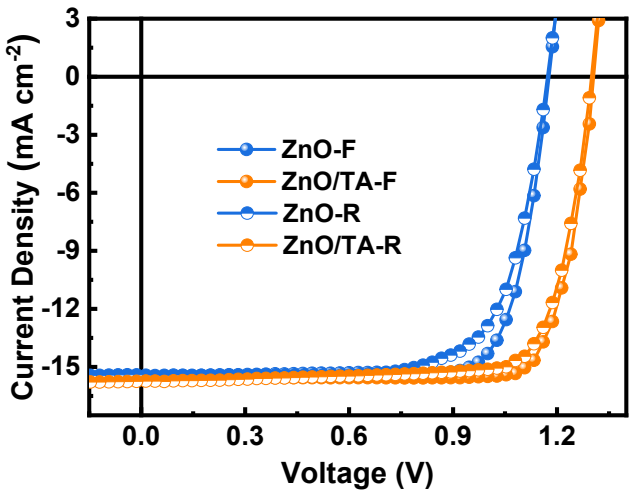

Fig. S6 *J-V* curves in the forward scan and reverse scan direction of the device based on bare ZnO and ZnO/TA ETLs, respectively.

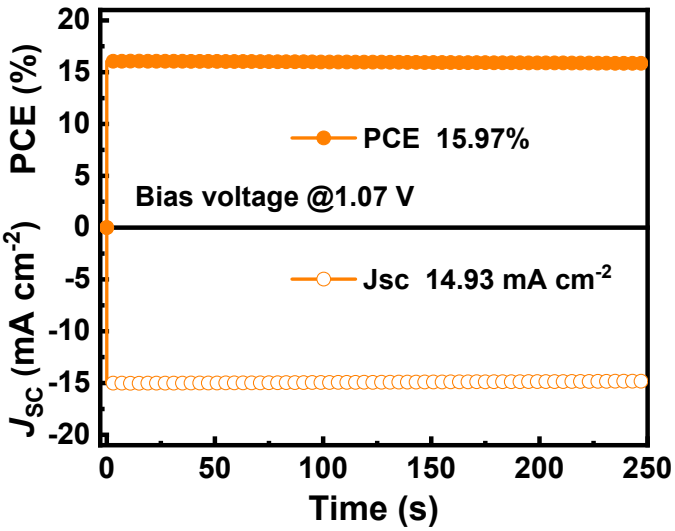

Fig. S7 The stabilized maximum power output of the device with ZnO/TA ETL.

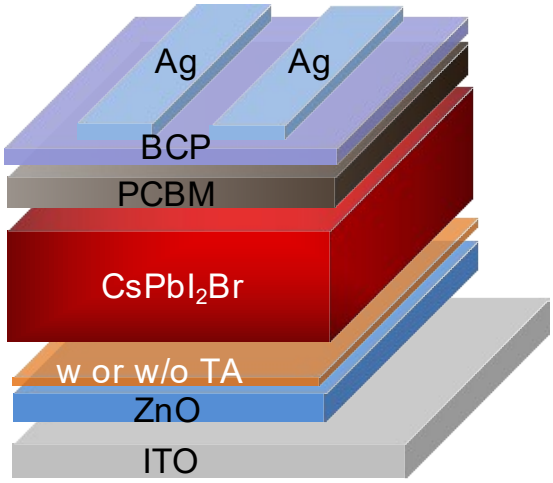

Fig. S8 Schematic illustration of the electron-only device structure of ITO/ETL/$CsPbI_2Br$/ PCBM/BCP/Ag for SCLC measurement.

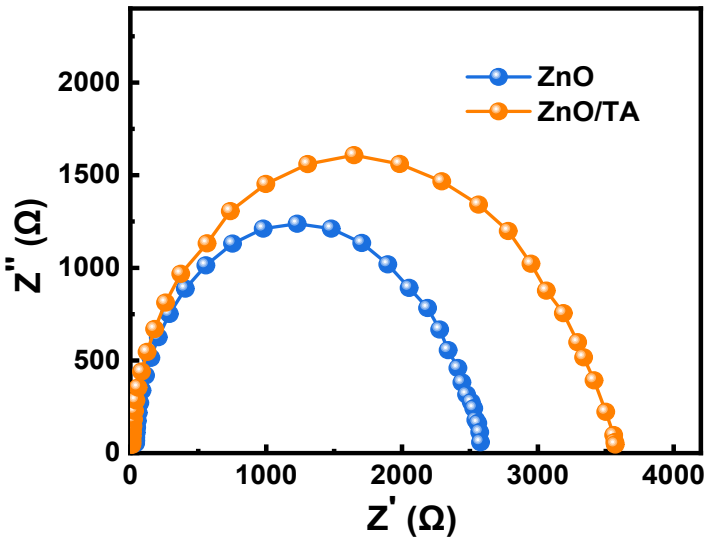

Fig. S9 EIS curves of PSCs based on ZnO and ZnO/TA ETLs.

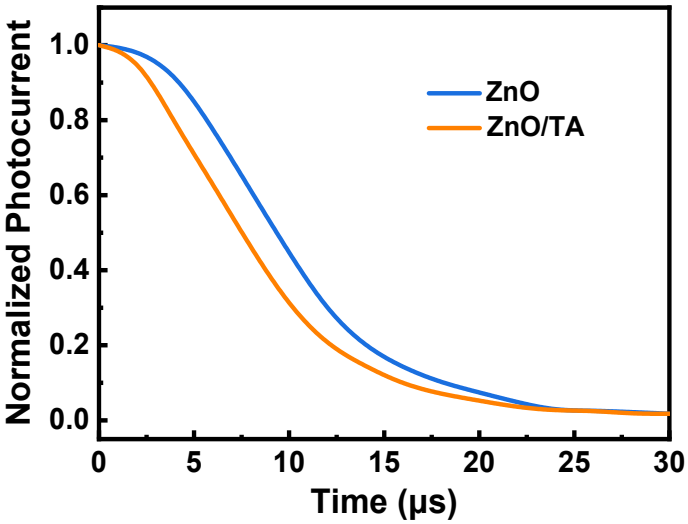

Fig. S10 TPC results of the $CsPbI_2Br$ PSCs using ZnO, and ZnO/TA as ETL.

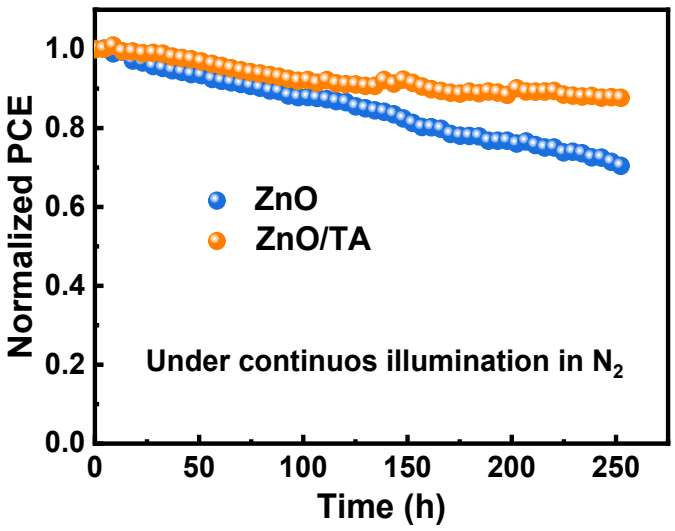

Fig. S11 Operational stability of the $CsPbI_2Br$ devices under continuous illumination in N_2 -filled glovebox.