

Efficient inverted CsPbI₃ inorganic perovskite solar cells achieved by facile surface treatment with ethanolamine

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Experimental Section

Materials: Lead iodide (PbI_2 , 99.9%), Cesium iodide (CsI , 99.9%), Dimethylamine hydroiodide (DMAI, 99%), [6,6]-phenyl-C61-butyric acid methyl ester (PCBM), and 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP) were purchased from Xi'an Polymer Light Technology Corp. Poly[3-(4-carboxylbutyl)thiophene (P3CT, Mw:30-40 k) was bought from the Rieke Metals. Isopropanol (IPA, 99%), dimethyl sulfoxide (DMSO, 99.8%, anhydrous), N-dimethylformamide (DMF, 99.8%), Ethanolamine (EA, 99.5%), chlorobenzene (CB, 99.9%) were purchased from Aladdin. All materials and reagents were used as received without further purification.

The preparation of CsPbI_3 precursor: Dissolve 156 mg CsI , 276.6 mg PbI_2 , and 103.8 mg DMAI in 1 mL DMF to obtain 0.6 M CsPbI_3 precursor. Then, the obtained precursor solutions were stirred at 45 °C for 2 h.

Device fabrication: The etched FTO glass substrates were ultrasonically cleaned by deionized water, ethanol, deionized water, and ethanol in turn for 15 min. Then the drying substrates were treated with ultraviolet ozone cleaner for 15 min to form a hydrophilic surface. Dissolve 10 mg of P3CT with 1 mL of methanol and add 67 μL of methylamine solution and stirred 45 °C for 15 min to obtain 10 mg/mL of P3CT-N. 1 mg/mL P3CT-N layer was spin-coated with 4000 rpm for 40 s on FTO and annealed at 100 °C for 10 min. Afterward, the substrates were transferred to the glove box. The perovskite precursor was preheated at 70 °C for 2 min and then deposited on the preheated FTO/P3CT-N by 3000 rpm for 30 s and annealed at 200 °C for 5 min to form a photovoltaic phase in an N_2 filled glove box. Next, 30 μL EA (the solvent isopropanol) was spin-coated on upper perovskite film at 3000 rpm for 30 s and annealed at 80 °C for 2 min. 20 mg/mL PCBM was spin-coated on the film at 3000 rpm for 30 s and

isopropanol saturated solution of BCP was spin-coated at 6000 rpm for 30 s. Finally, a 100 nm-thick Ag electrode was deposited by thermal evaporation to complete the cell. The effective device area was defined to be 0.08 cm² controlled with a metal mask.

Characterizations: X-ray diffraction patterns (XRD, Bruker D8 Advance instrument with Cu K α X-ray radiation about 0.154 nm) were used to test crystal structure and diffraction angle range from 5° to 45°. The morphology characterization of the films was measured by SEM (JSM-7800F). The surface morphology of the perovskite films was tested by atomic force microscopy (AFM, Asylum Research Cypher, UK). PL and TRPL spectra were recorded using the FluoTime 300 fluorescence lifetime spectrometer (PicoQuant). The chemical states were tested by X-ray photoelectron spectroscopy (XPS, Kratos Axis Ultra DLD) using Al K α as radiation, and the C 1s line at 284.6 eV was used for correction all spectra. The UPS measurements were performed with a He I ($h\nu = 21.22$ eV) gas discharge lamp for excitation and a total instrumental energy resolution of 100 meV and samples were negatively biased for the observation of SECOs. The J - V curves were collected by a calibrated solar simulator (Newport Inc.) with an AM 1.5G filter and Keithley 2400 source meter under 100 mW/cm² in the glove box. The voltage scanning range was from 2 V to -0.2 V with a dwell time of 50 ms. The space-charge-limited current (SCLC) measurements and dark J - V curves were measured by the Keithley 4200 m under dark conditions. The transient photo-current (TPC) decay and transient photo-voltage (TPV) decay were recorded by an electrochemical workstation (Zahner, Germany) with a white light LED supplied 80

Mw/cm² light intensity to excite the perovskite solar cells. The external quantum efficiency (EQE) was tested by the Newport EQE system and the wavelength ranged from 300 to 800 nm.

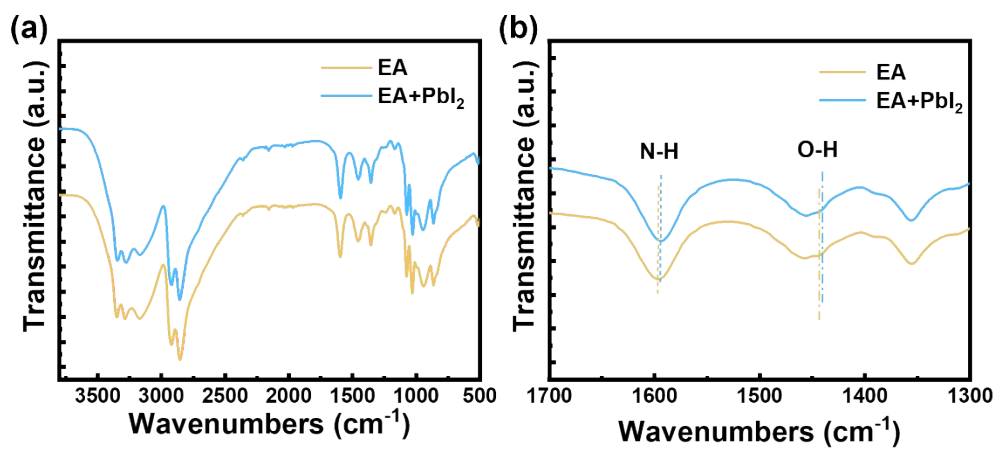


Fig. S1 (a) The full FTIR spectroscopy of EA and EA+PbI₂. (b) FTIR spectroscopy of (C-OH) and (N-H) groups.

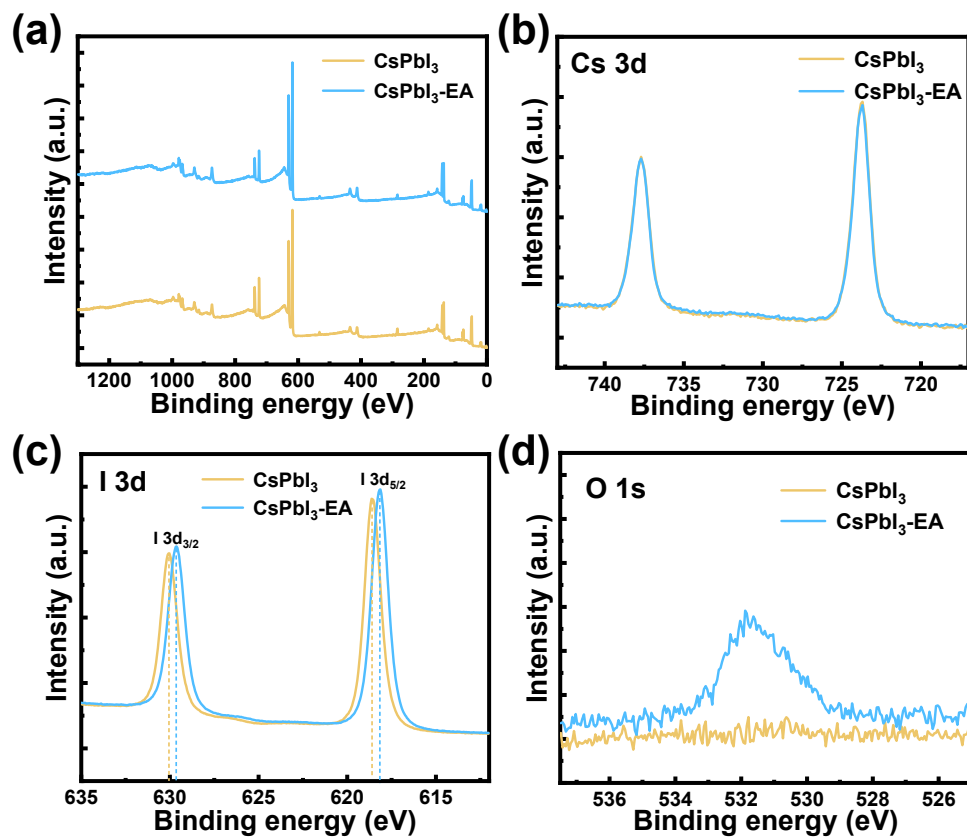


Fig. S2 (a) Full-scan XPS spectra. (b) XPS spectra of Cs 3d, (c) I 3d and (d) O 1s.

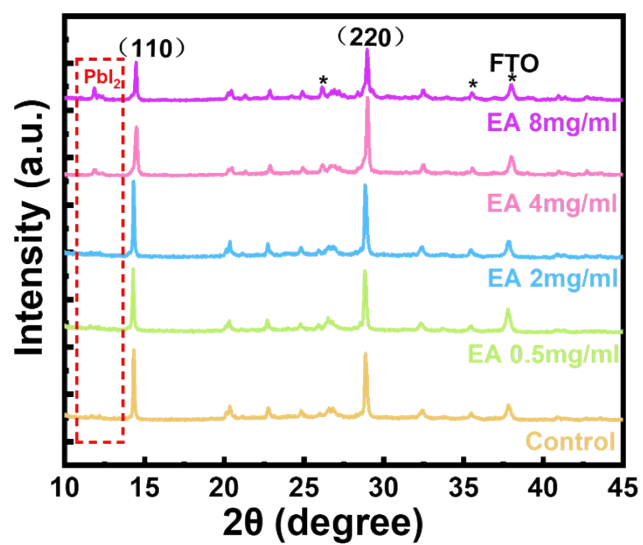


Fig. S3 XRD patterns of CsPbI₃ film based on EA treatment with different concentrations.

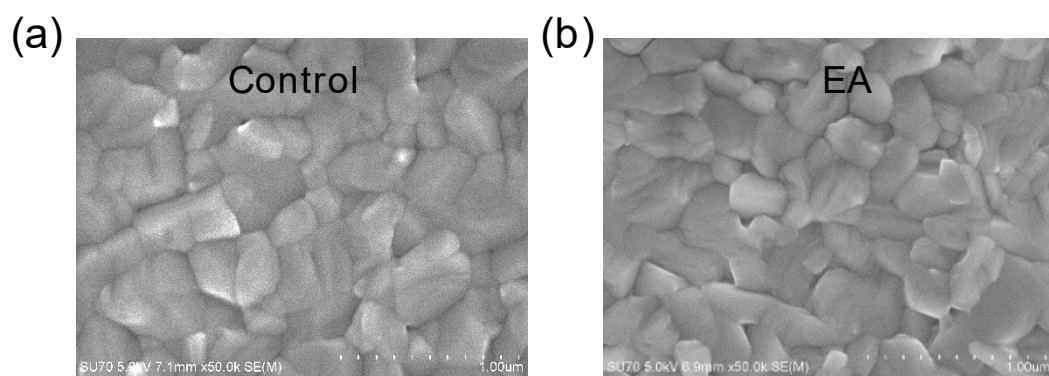


Fig. S4 High-resolution top-view SEM images of the (a) control CsPbI₃ perovskite film, (b) EA-treated CsPbI₃ film.

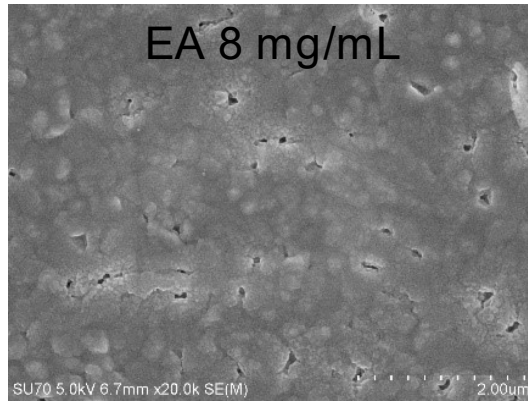


Fig. S5 SEM image of CsPbI₃ film treated with a high concentration of 8 mg/mL EA.

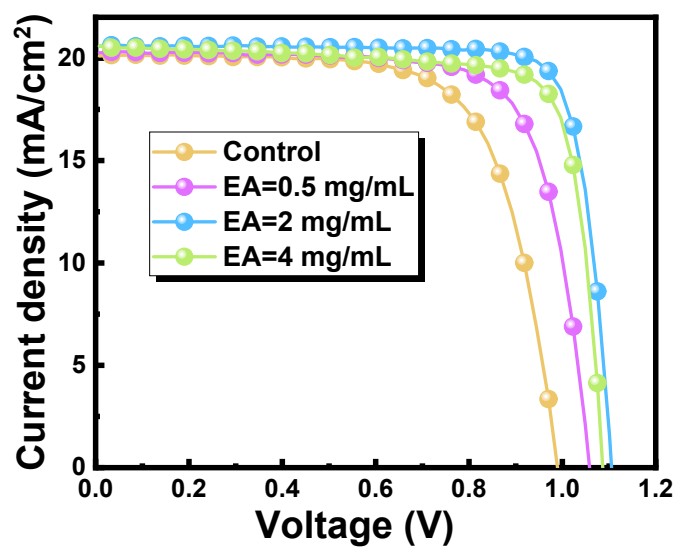


Fig. S6 J - V curves of devices treated with different EA concentrations (0, 0.5, 2, and 4 mg/mL).

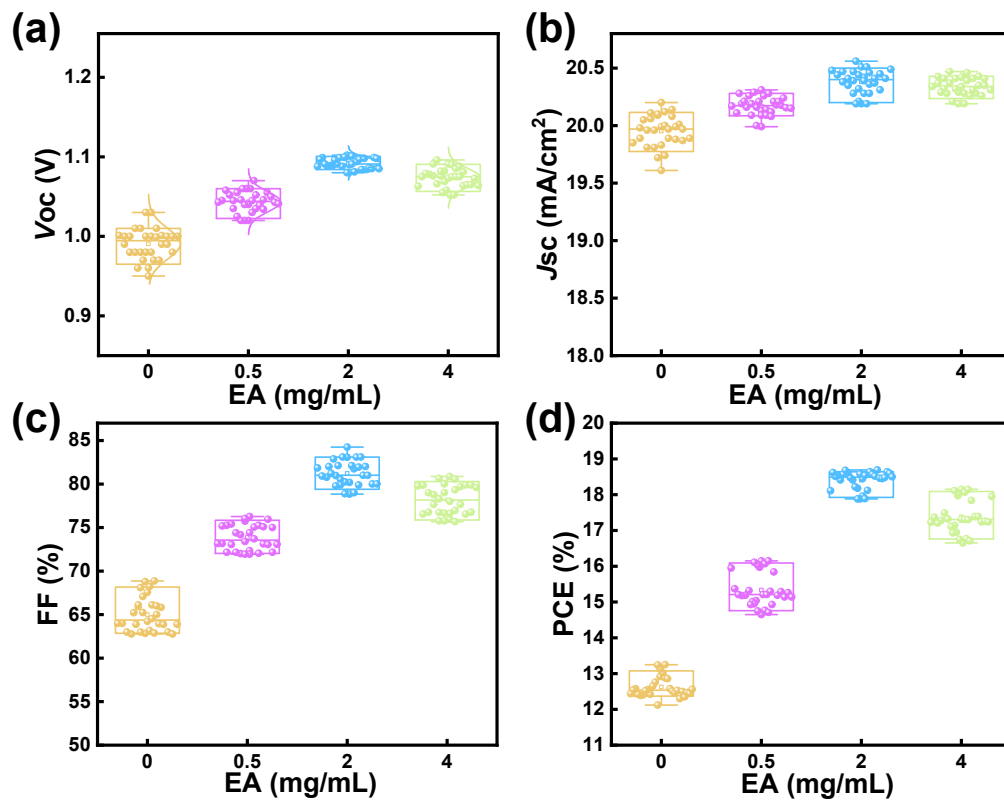


Fig. S7 Box statistics of (a) V_{oc} , (b) J_{sc} , (c) FF, and (d) PCE with different EA concentrations.

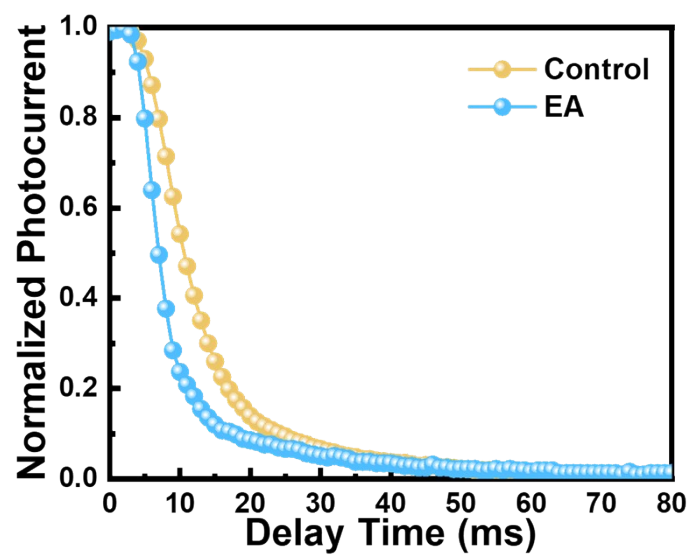


Fig. S8 Transient photocurrent testing of devices.

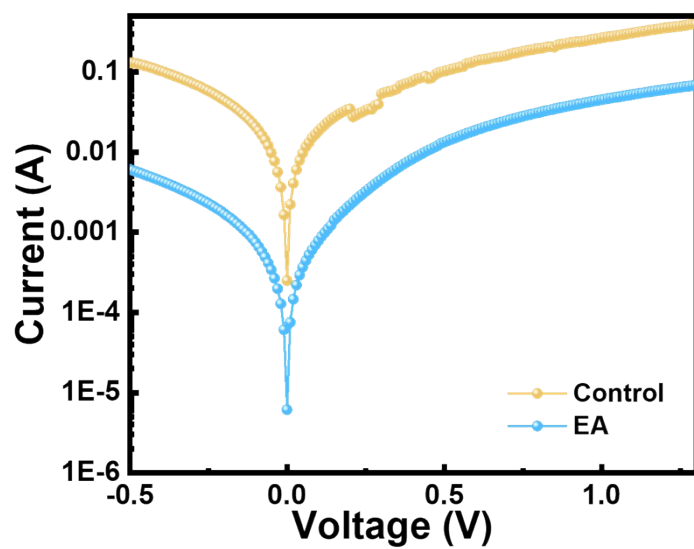


Fig. S9 The dark current curve of the devices.

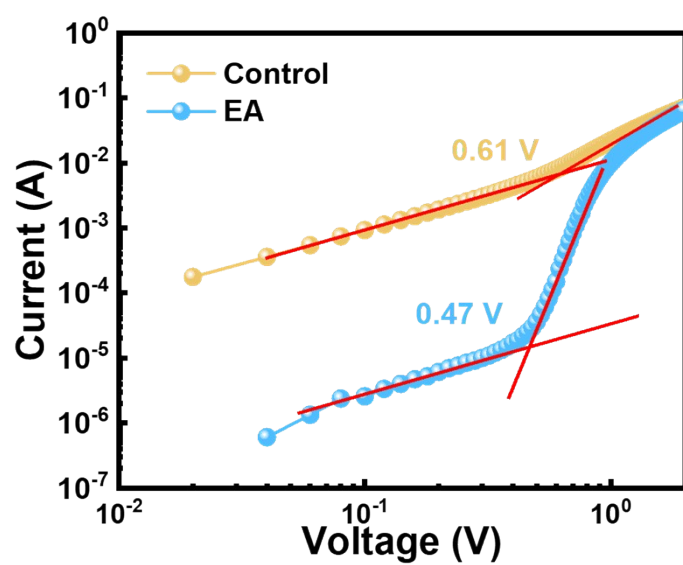


Fig. S10 The space-charge-limited current (SCLC) curves of hole-only devices.

Table S1. Photovoltaic parameters of devices treated with different EA concentrations.

Device	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
Control	0.991	20.14	64.87	12.95
EA 0.5 mg/mL	1.033	20.20	73.96	15.43
EA 2 mg/mL	1.112	20.51	80.68	18.41
EA 4 mg/mL	1.082	20.38	80.03	17.65

Table S2 Photovoltaic parameters of the PSCs from forward and reverse scanning J - V curves.

Device	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
Control-F	0.991	20.14	64.87	12.95
Control-R	0.872	19.51	57.14	9.72
EA-F	1.112	20.51	80.68	18.41
EA-R	1.041	20.55	77.21	16.52

Table S3 The specific fitted parameters of EIS curves of the CsPbI₃ PSCs.

Device	R_s (Ω)	R_{tr} (Ω)	C_{tr} (F)	R_{rec} (Ω)	C_{rec} (F)
Control	28.5	244.6	1.56×10^{-5}	1857	2.39×10^{-8}
EA	23.1	77.4	1.01×10^{-5}	3992	1.71×10^{-8}