

Supporting information

Suppressing the penetration of 2D perovskites for enhanced stability of perovskite solar cells

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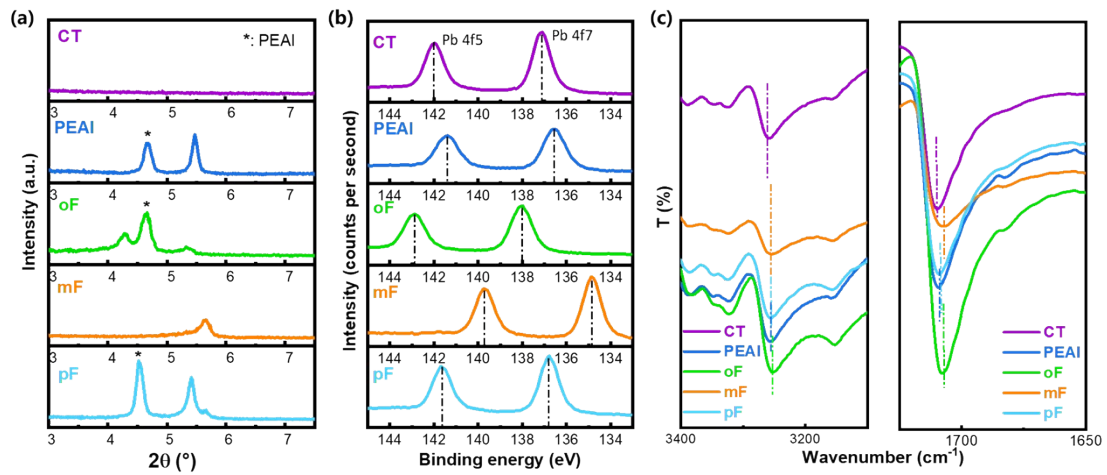


Figure S1. (a) X-ray diffraction patterns, (b) Pb4f XPS spectra, and (c) FTIR spectra of the control perovskite film, PEAI-treated film and o/m/p-FPEAI-treated films.

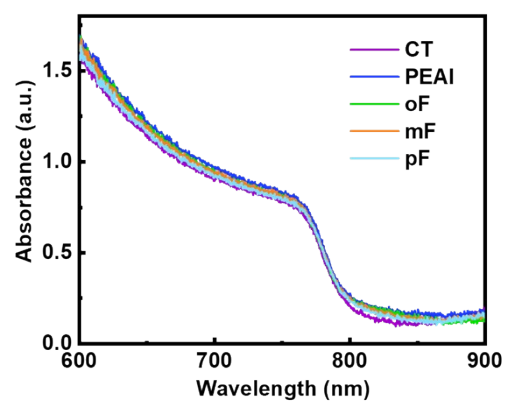


Figure S2. UV-vis spectra of the control perovskite film, PEAI-treated film and o/m/p-FPEAI-treated films.

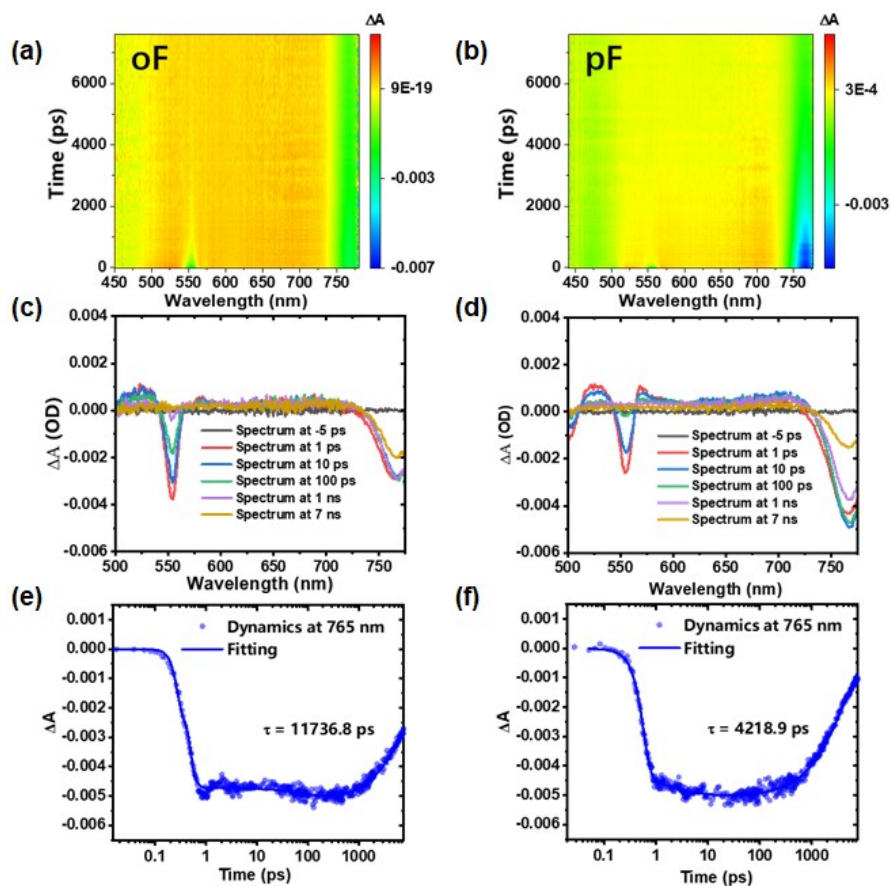


Figure S3. (a-b) Contour plot TA spectra; (c-d) TA spectra at various decay time; (e-f) decay curves of the bleaching peak at 765 nm for perovskite films modified with (a, c, e) o-FPEAI and (b, d, f) p-FPEAI.

Table S1. Carrier lifetimes of the control perovskite film, PEAI-treated film and o/m/p-FPEAI-treated films.

	A1	T1 (ps)	A2	T2 (ps)	A3	T3 (ps)	R²
CT	3.3E-4	2.1E-1	-2.8E-4	6.3	-2.7E-3	5462.1	0.995
PEAI	8.8E-4	134.6	-6.5E-4	134.6	-1.3E-3	5101.4	0.994
oF	4.4E-4	8.7E-2	1.2	103.5	-1.5E-3	11736.8	0.996
mF	2.7E-3	10.9	-2.7E-3	10.4	-1.8E-3	15341.6	0.996
pF	2.2E-3	1.2	1.1	6.9	-2.4E-3	4218.9	0.996

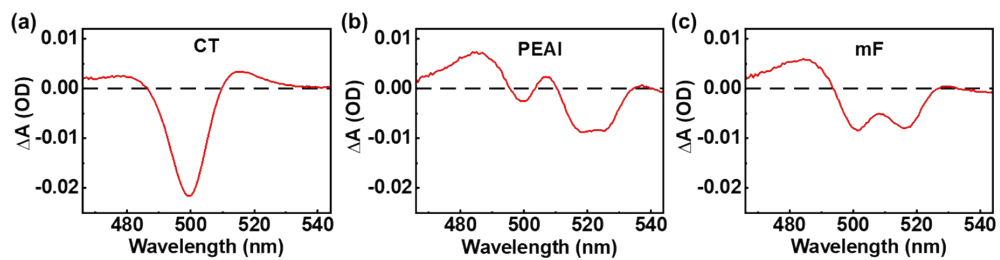


Figure S4. (a-c) Transient Absorption spectra of (a) control PbI₂ film, (b) PEAI-treated PbI₂ film, and (c) m-FPEAI-treated PbI₂ film.

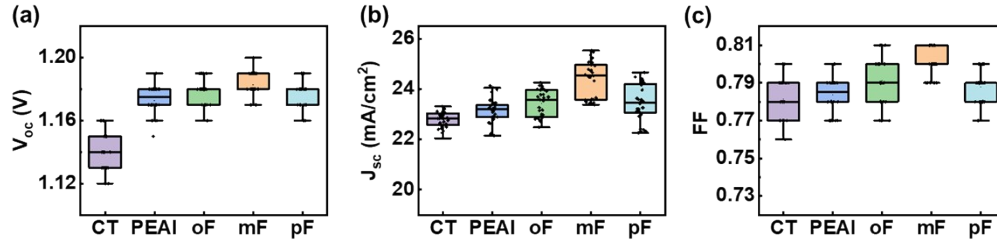


Figure S5. Photovoltaic parameter distribution for five groups of PSCs with the composition of $\text{Cs}_{0.05}\text{FA}_{0.88}\text{MA}_{0.07}\text{PbI}_{2.79}\text{Br}_{0.21}$. **(a)** Open-circuit voltage (V_{oc}). **(b)** Short-circuit current density (J_{sc}). **(c)** Fill factor (FF).

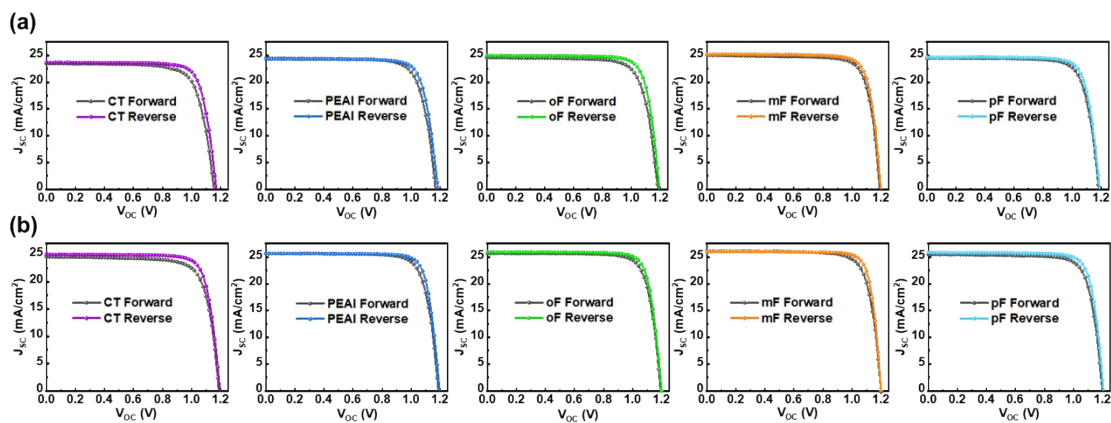


Figure S6. The forward and reverse scan curves of the control PSC, PEAI-treated PSC, and o/m/p-FPEAI-treated PSCs with the composition of **(a)** $\text{Cs}_{0.05}\text{FA}_{0.88}\text{MA}_{0.07}\text{PbI}_{2.79}\text{Br}_{0.21}$ and **(b)** $\text{Cs}_{0.05}\text{FA}_{0.92}\text{MA}_{0.03}\text{PbI}_{2.91}\text{Br}_{0.09}$.

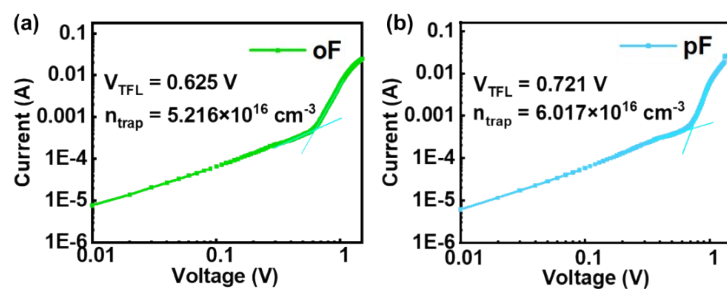


Figure S7. Space-charge-limited current (SCLC) curves for **(a)** o-FPEAI-treated PSC, and **(b)** p-FPEAI-treated PSC.

Device Fabrication:

ITO substrates were cleaned with detergent, deionized water, acetone and ethanol in sequential and treated with UV Ozone before use. SnO₂ layer was deposited by spin coating the commercially SnO₂ colloidal solution (2.5 wt % in H₂O) at 3000 rpm for 40 s followed by heating at 150 °C for 30 minutes. The perovskite with the formula of (CsPbI₃)_{0.05}(MAPbBr₃)_{0.07}(FAPbI₃)_{0.88} were dissolved in the mix solvents of DMF and DMSO with the volume ratio of 7:3. Besides, MACl was added in with a concentration of 15 mg/ml. The precursor solution was spin coated onto SnO₂ at 3000 rpm for 10 s and 6000 rpm for 30 s. 500 µL toluene was dropped on to the spinning film at the 15th second. The as deposited film was annealed at 100 °C for 30 minutes. To deposit the modification layer, PEAI or ortho-, meta-, para-FPEAI (o/m/p-FPEAI) was dissolved in IPA with a concentration of 4 mg/ml and spin coated on the surface of perovskite films at 6000 rpm for 60 s.

The optimized perovskite of (CsPbI₃)_{0.05}(MAPbBr₃)_{0.03}(FAPbI₃)_{0.92} were dissolved in the mix solvents of DMF and DMSO with the volume ratio of 89:11. Besides, MACl was added in with a concentration of 34 mg/ml. The precursor solution was spin coated onto SnO₂ at 1000 rpm for 10 s and 4000 rpm for 30 s. 800 µL ether was dropped on to the spinning film at the 15th second. The as deposited film was annealed at 100 °C for 40 minutes.

To prepare the spiro-OMeTAD solution, 90.0 mg Spiro-OMeTAD powder, 28.5 µL 4-tBP and 17.5 µL Li-TFSI solution (260 mg of Li-TFSI powder dissolved in 1 mL acetonitrile) were dissolved in 1 ml CB. The spiro-OMeTAD layer was deposited by spin coating the solution at 3000 rpm for 30 s. Finally, 80 nm gold electrode was evaporated via a mask.

Characterization

SEM images were tested by LEO 1530 Field Emission Scanning Electron Microscope. AFM images were tested with Bruker MultiMode 8 Atomic Force Microscope. XRD patterns were tested by Bruker D8 Advance X-Ray Diffractometer.

XPS spectra were tested by a spectroscope (SPECS, Germany). UV-vis optical absorption spectra were recorded using a spectroscope (JASCO V-770EX, Japan). JV curves were collected by a source meter (Keithley 2400, Tektronix, USA) in combination with a solar simulator. PL spectra were tested by a spectrometer (Acton SpectraPro SP-2300, Teledyne Princeton Instruments, USA). TA spectra were measured with the HELIOS TA system.