

Supporting information

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

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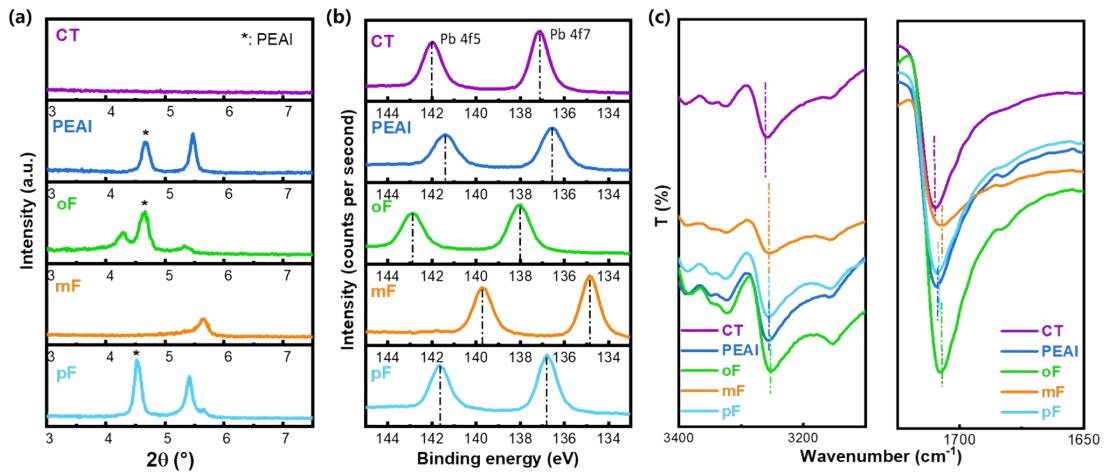


Figure S1. (a) X-ray diffraction patterns, (b) Pb4f XPS spectra, and (c) FTIR spectra of the control perovskite film, PEAi-treated film and o/m/p-FPEAI-treated films.

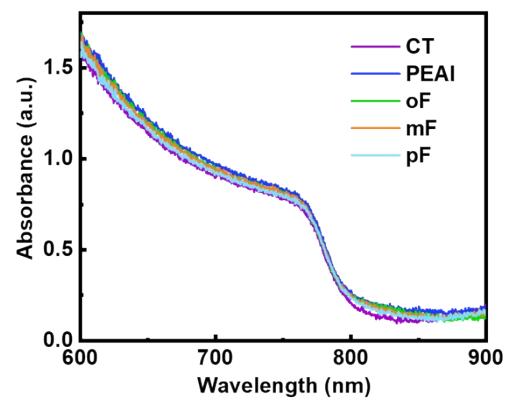


Figure S2. UV-vis spectra of the control perovskite film, PEAI-treated film and o/m/p-FPEAI-treated films.

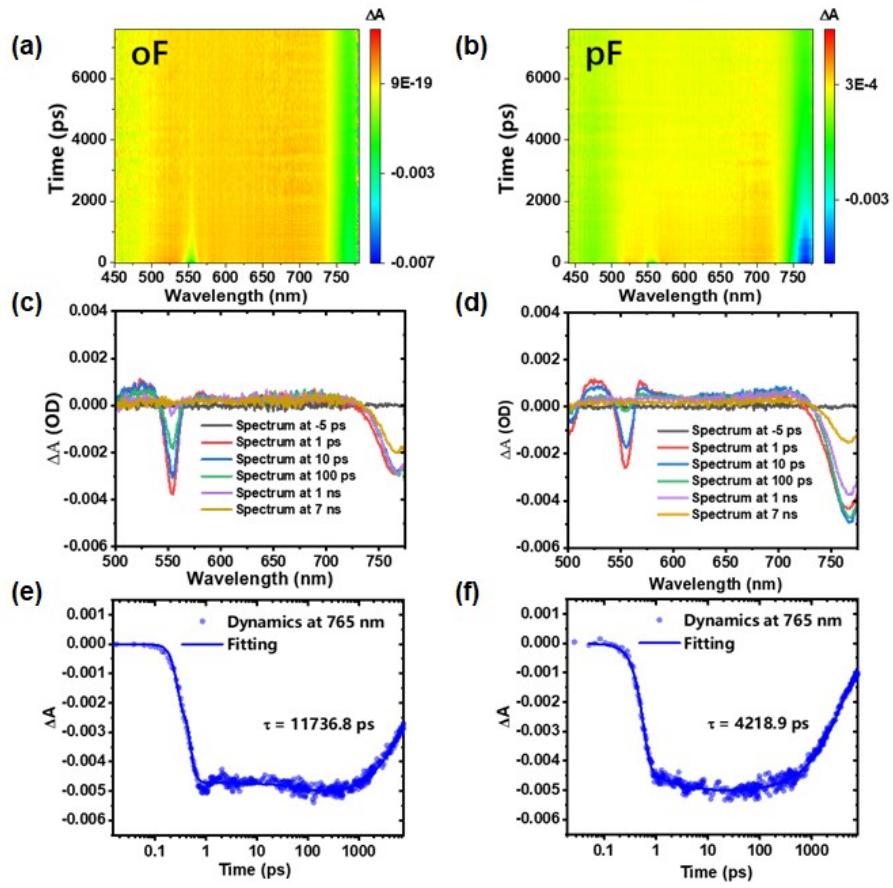


Figure S3. (a-b) Contour plot TA spectra; (c-d) TA spectra at various decay time; (e-f) decay curves of the bleaching peak at 765 nm for perovskite films modified with (a, c, e) o-FPEAI and (b, d, f) p-FPEAI.

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 |

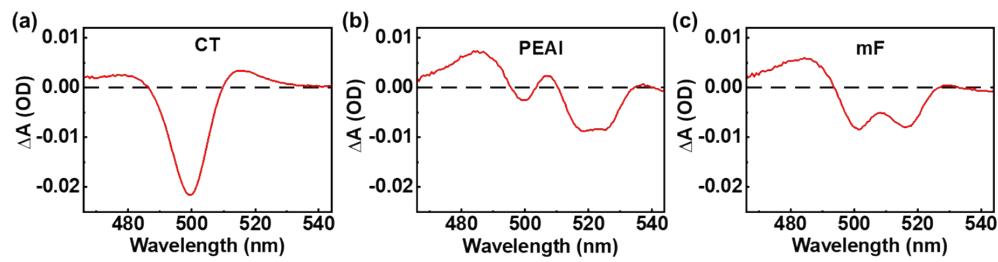


Figure S4. (a-c) Transient Absorption spectra of (a) control PbI₂ film, (b) PEAI-treated PbI₂ film, and (c) m-FPEAI-treated PbI₂ film.

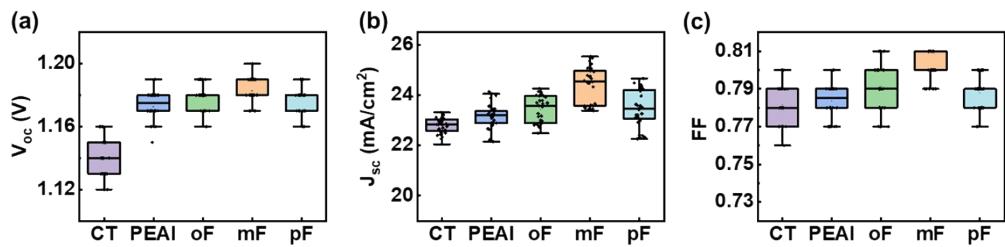


Figure S5. Photovoltaic parameter distribution for five groups of PSCs with the composition of $\text{Cs}_{0.05}\text{FA}_{0.88}\text{MA}_{0.07}\text{PbI}_{2.79}\text{Br}_{0.21}$. **(a)** Open-circuit voltage (V_{oc}). **(b)** Short-circuit current density (J_{sc}). **(c)** Fill factor (FF).

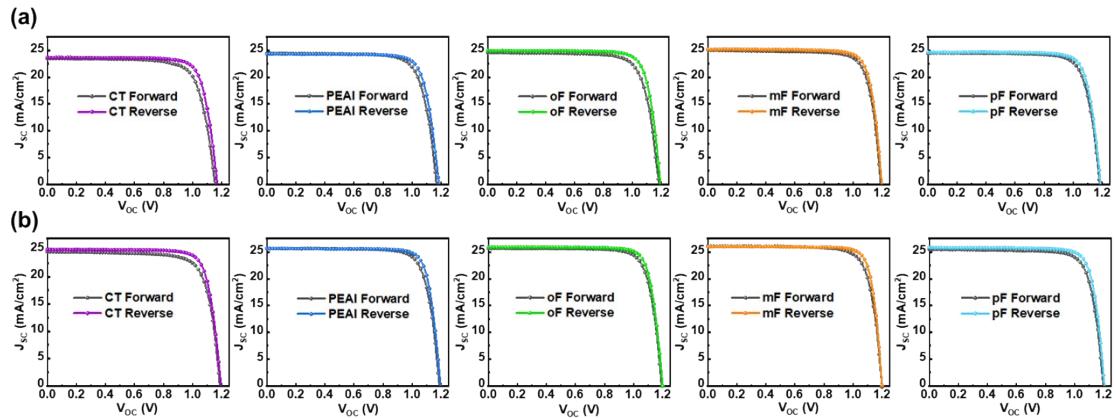


Figure S6. The forward and reverse scan curves of the control PSC, PEAI-treated PSC, and o/m/p-FPEAI-treated PSCs with the composition of (a) $\text{Cs}_{0.05}\text{FA}_{0.88}\text{MA}_{0.07}\text{PbI}_{2.79}\text{Br}_{0.21}$ and (b) $\text{Cs}_{0.05}\text{FA}_{0.92}\text{MA}_{0.03}\text{PbI}_{2.91}\text{Br}_{0.09}$.

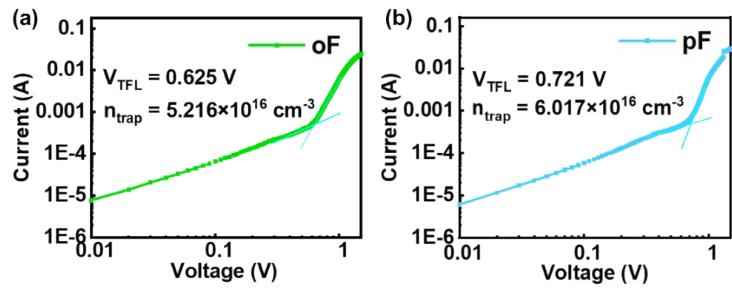


Figure S7. Space-charge-limited current (SCLC) curves for (a) o-FPEAI-treated PSC, and (b) p-FPEAI-treated PSC.

Device Fabrication:

ITO substrates were cleaned with detergent, deionized water, acetone and ethanol in sequential and treated with UV Ozone before use. SnO_2 layer was deposited by spin coating the commercially SnO_2 colloidal solution (2.5 wt % in H_2O) at 3000 rpm for 40 s followed by heating at 150 °C for 30 minutes. The perovskite with the formula of $(\text{CsPbI}_3)_{0.05}(\text{MAPbBr}_3)_{0.07}(\text{FAPbI}_3)_{0.88}$ were dissolved in the mix solvents of DMF and DMSO with the volume ratio of 7:3. Besides, MCl was added in with a concentration of 15 mg/ml. The precursor solution was spin coated onto SnO_2 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 $(\text{CsPbI}_3)_{0.05}(\text{MAPbBr}_3)_{0.03}(\text{FAPbI}_3)_{0.92}$ were dissolved in the mix solvents of DMF and DMSO with the volume ratio of 89:11. Besides, MCl was added in with a concentration of 34 mg/ml. The precursor solution was spin coated onto SnO_2 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.