

Supplementary Materials

Reconstructing the perovskite surface with a homogeneous electric potential by reducing localized charge for efficient and durable perovskite solar cells

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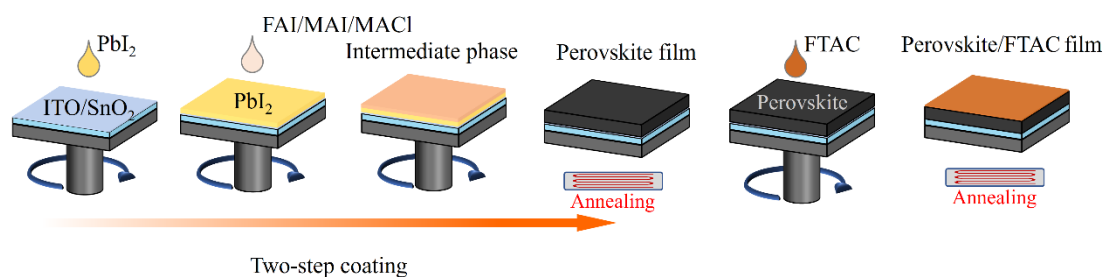


Figure S1. Image of process for preparing solar cells and passivation layer.

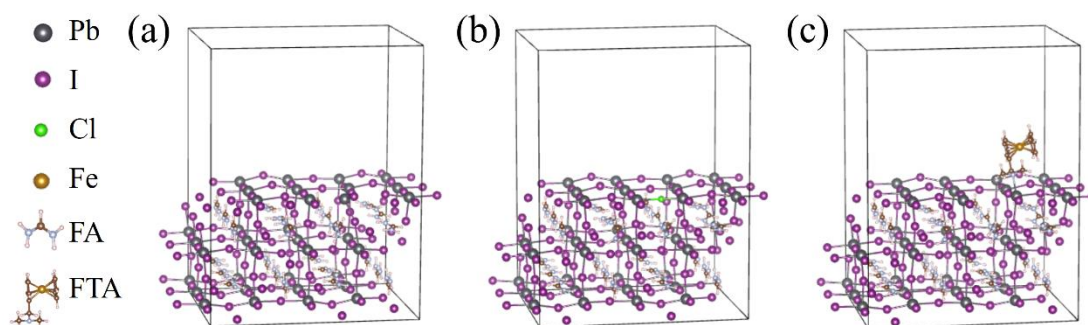


Figure S2. DFT models constructed to investigate the surface passivation mechanism of FTAC on FAPbI₃: a) V₁-FAPbI₃ surface, b) Cl-passivated FAPbI₃ surface, and c) FTA-modified FAPbI₃ surface.

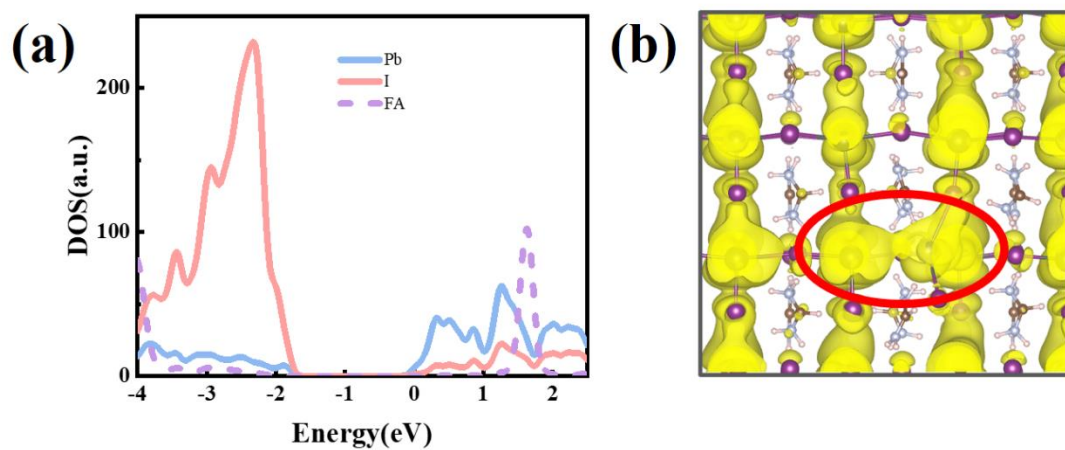


Fig.S3. a-b) Density of state and charge density distribution of V₁-FAPbI₃ system.

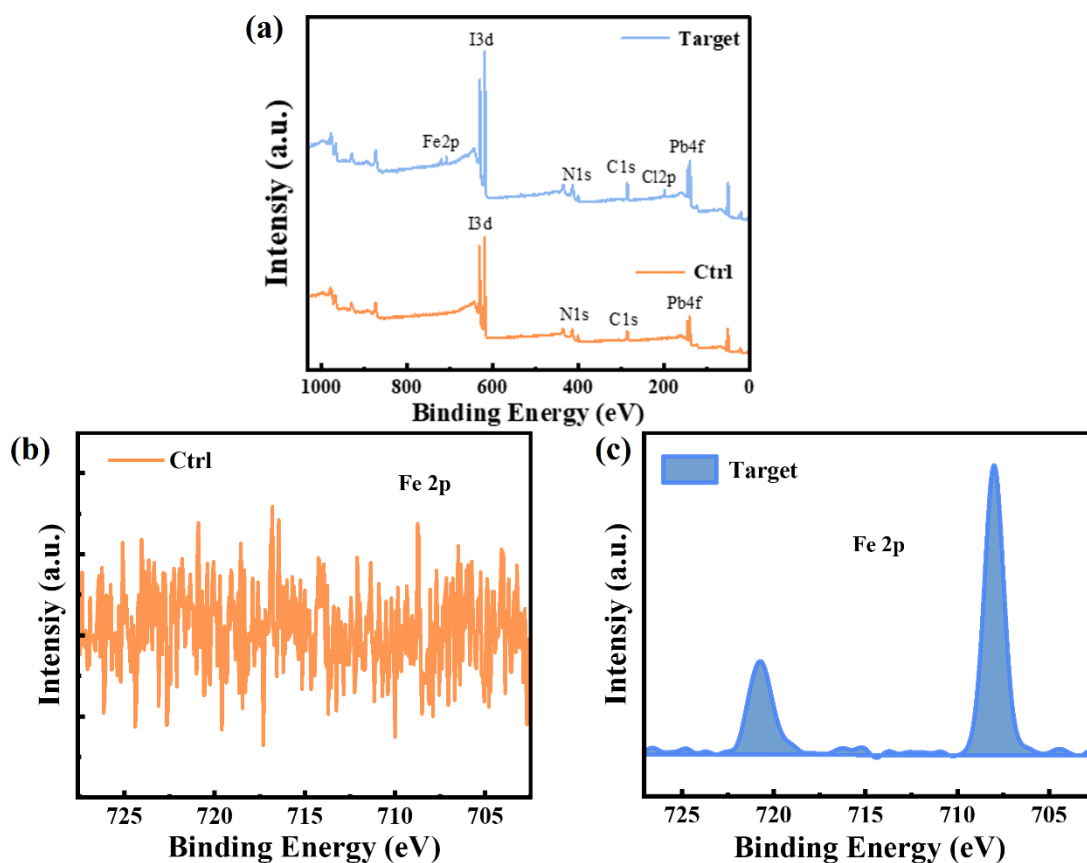


Figure S4. a) XPS spectra of the pristine and FTAC-modified perovskite films, high-resolution Fe 2p regions for c) pristine and d) modified perovskite layers.

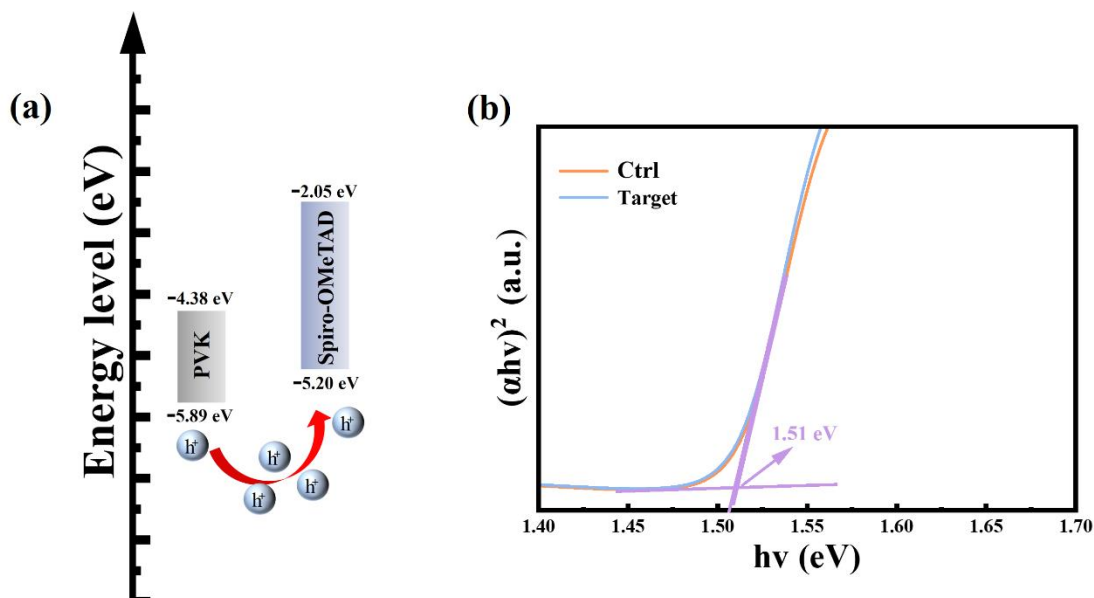


Figure S5. a) Energy level diagram of the control perovskite layer and hole transport layer. b) Tauc plot spectra of the control and target perovskite films.

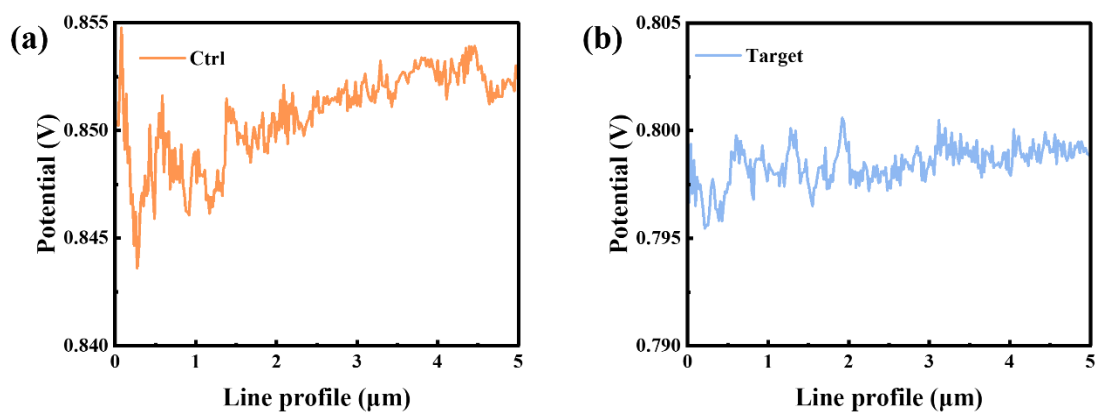


Figure S6. The CPD line-scan profiles of the a) control and b) target perovskite films.

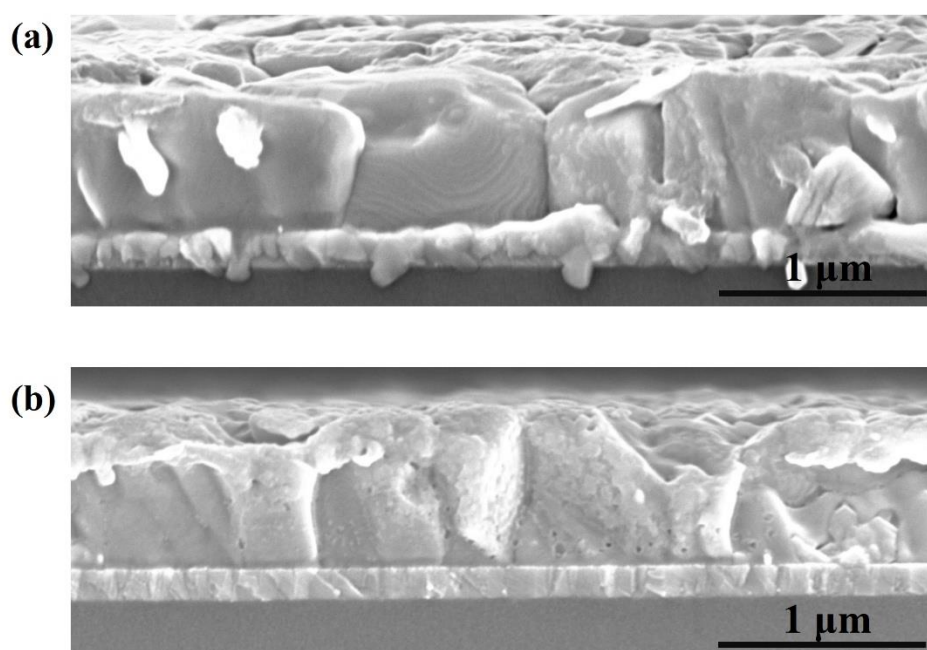


Figure S7. Cross-sectional SEM images for a) the control and b) the target films.

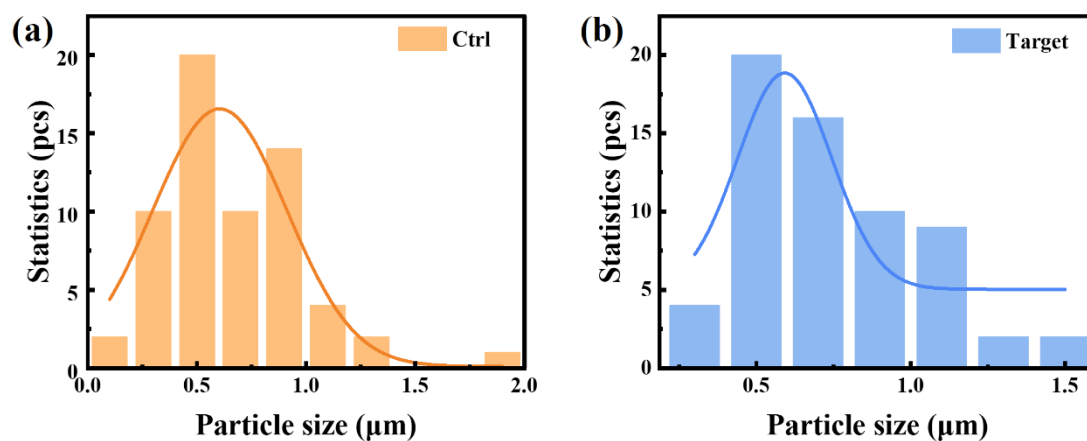


Figure S8. The grain size statistics chart of a) control and b) target perovskite films.

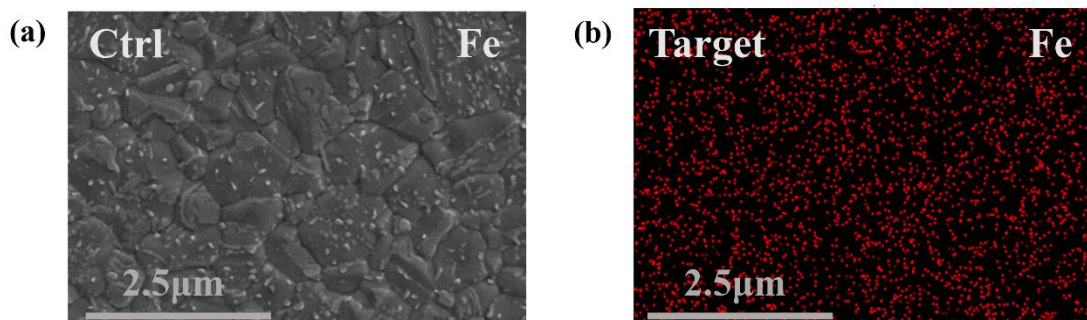


Figure S9. EDS images of the a) control and b) target perovskite films.

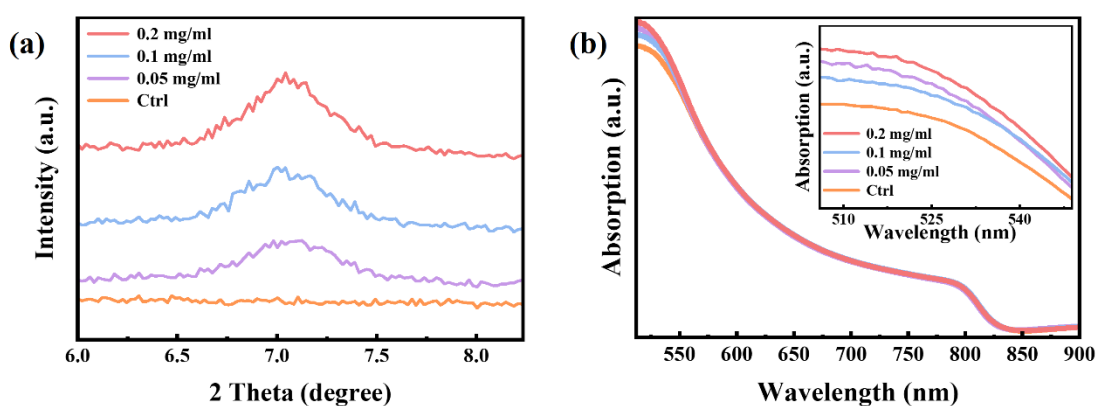


Figure S10. a) The Low-angle XRD patterns of the control and FTAC modified perovskite films. b) The absorbance spectra of the control and FTAC modified perovskite films.

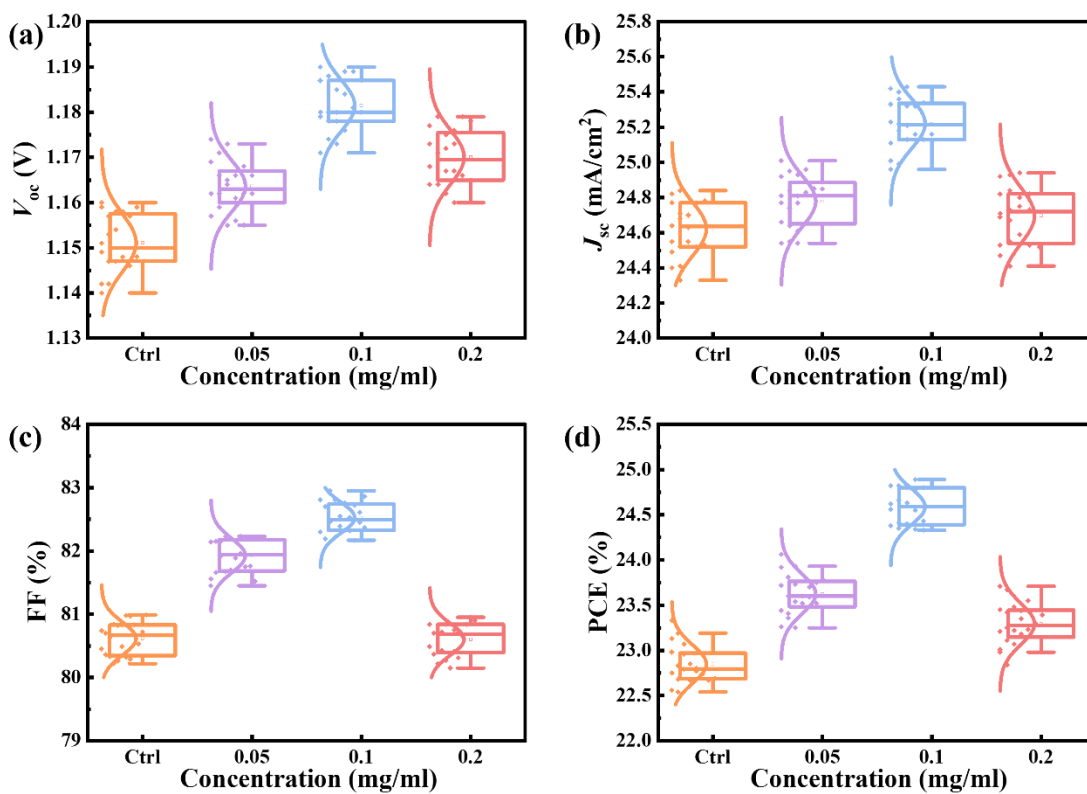


Figure S11. Statistics of key photovoltaic parameters (open-circuit voltage (V_{oc}), fill factor (FF), short-circuit current density (J_{sc}), PCE) obtained from the J - V characteristic of 20 control

devices, and devices modified with different concentrations of FTAC (0.5, 1.0 and 2.0 mg/ml). The average value and standard deviation of each parameter is summarized in Table S5.

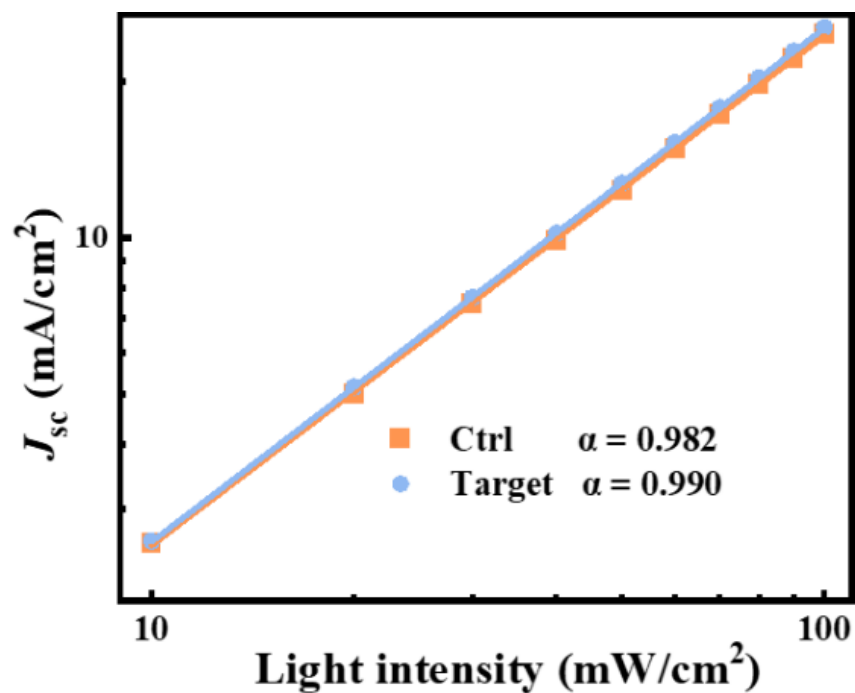


Figure S12. J_{sc} dependence on light intensity from 10 to 100 mW/cm^2 of different PSCs.

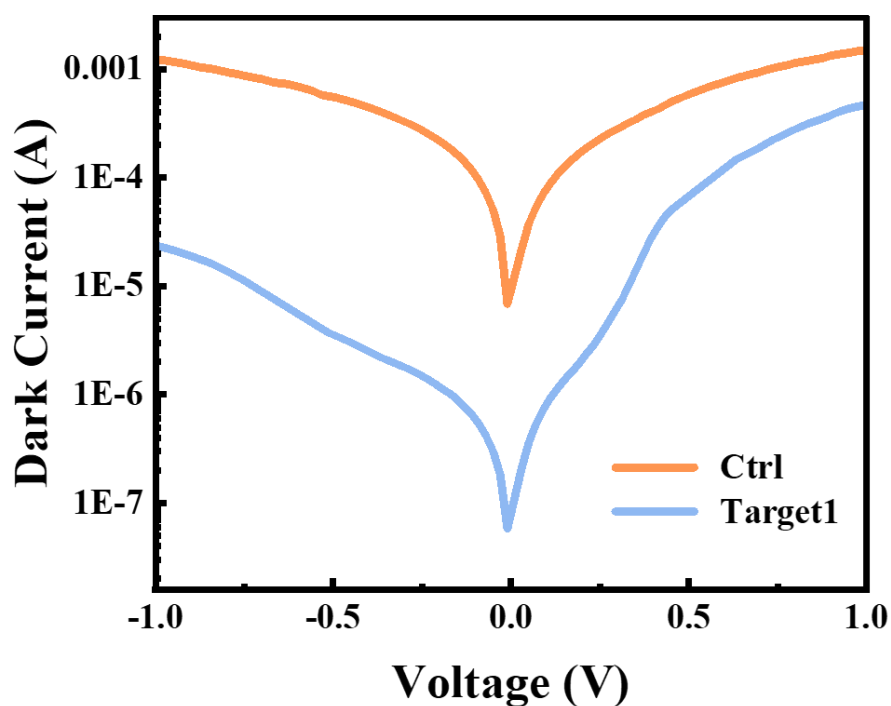


Figure S13. J - V curves of control and target PSCs under dark environment.

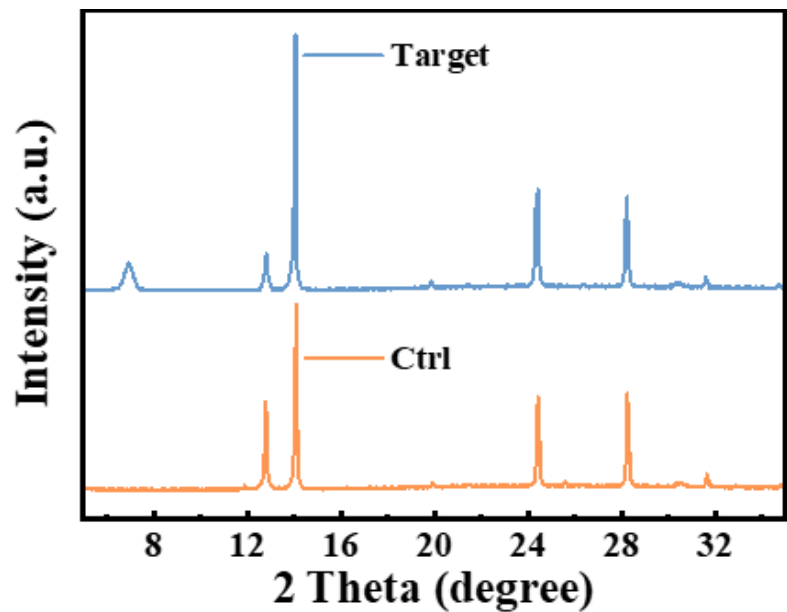


Figure S14. XRD characterization of the control and FTAC-modified perovskite films aged for 250 hours.

Table S1. XPS fitting results of the surface region of the perovskite

	Peak	Binding Energy (eV)	FWHM	Area (CPS·eV)	Atomic (%)
one-step	N 1s	400.60	1.19	21522.11	13.09
	Pb 4f7/2	138.34	1.06	160987.20	86.91
two-step	N 1s	400.88	1.18	21614.77	12.46
	Pb 4f7/2	138.59	1.03	171118.95	87.54

Table S2. XPS fitting results of the surface region of the perovskite

	Pb 4f / N 1s (Atomic)
one-step	6.64
two-step	7.02

Table S3. The KPFM data statistics of control and target perovskite films

Sample	Minimum(mV)	Maximum(mV)	Average value (mV)
Ctrl	812.4	855.94	855.95
Target	747.4	844.4	797.6

Table S4. XPS fitting results of the surface region of the perovskite

	Peak	Area (CPS·eV)	Atomic (%)
Control sample	I 3d	547029.11	84.99
	Pb 4f	124208.01	15.01
Optimized sample	I 3d	577658.40	85.18
	Pb 4f	129191.15	14.82

Table S5. Devices with different concentrations diffraction peak areas of (100) and (111) crystal planes and their ratio

Simple	13.78°	24.2°	Ratio
Ctrl	245.05	247.19	0.99
0.05mg/ml	268.11	225.93	1.19
Target	454.87	242.88	1.87
0.2mg/ml	523.02	314.47	1.66

Table S6. The statistic photovoltaic parameters of the control and optimized PSCs

Sample	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
Ctrl	1.151±0.008	24.62±0.15	80.62±0.25	22.85±0.21
0.05mg/ml	1.164±0.006	24.78±0.14	81.93±0.26	23.62±0.22
Target	1.181±0.005	25.22±0.14	82.52±0.24	24.59±0.19
0.2mg/ml	1.170±0.007	24.70±0.16	80.60±0.24	23.29±0.22