Supporting information

Efficient Surface Passivation of Perovskite Films by Post-treatment Method with a Minimal Dose

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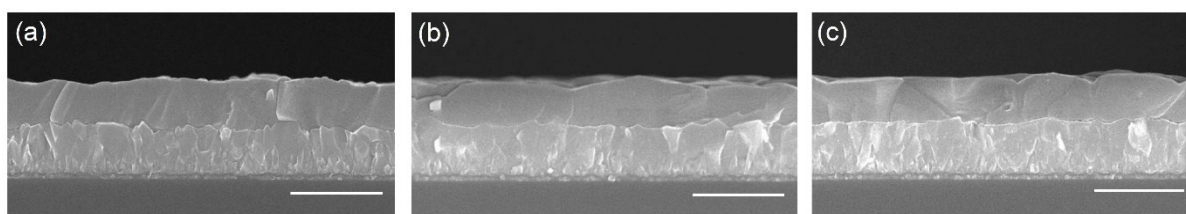
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Figure S1. Cross-sectional SEM image of (a) the reference film, (b) the film after APP-PT with 5.0 mM TBAI and (c) the film after UIP-PT with 0.05 mM TBAI. The films were formed on FTO substrate. Scale bar is 1 μm.
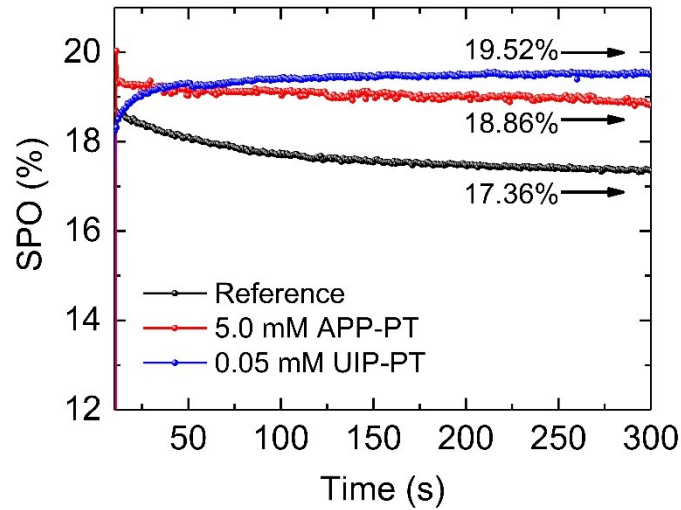
Figure S2. The steady-state power outputs (SPOs) of the reference, APP-PT and UIP-PT devices measured for 300 s at the maximum power points.
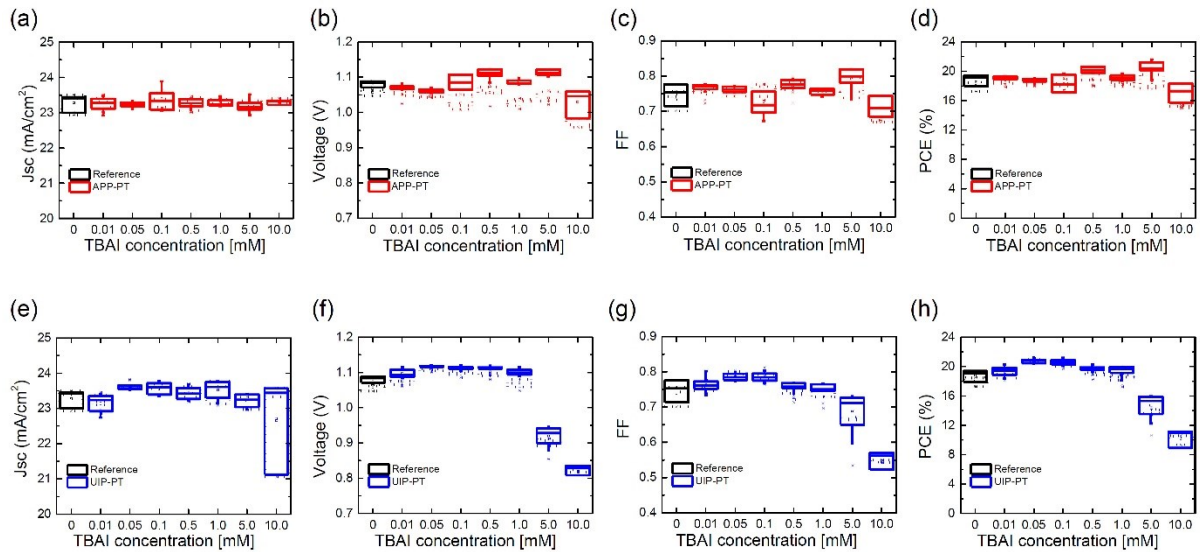

Figure S3. Statistical photovoltaic parameters of short-circuit photocurrent density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF) and power conversion efficiency (PCE) for the perovskite films after post-treatment by (a-d) APP-PT and (e-h) UIP-PT process depending on the TBAI concentration. Solid lines and dotted lines represent the reverse-scanned and forward-scanned data, respectively.
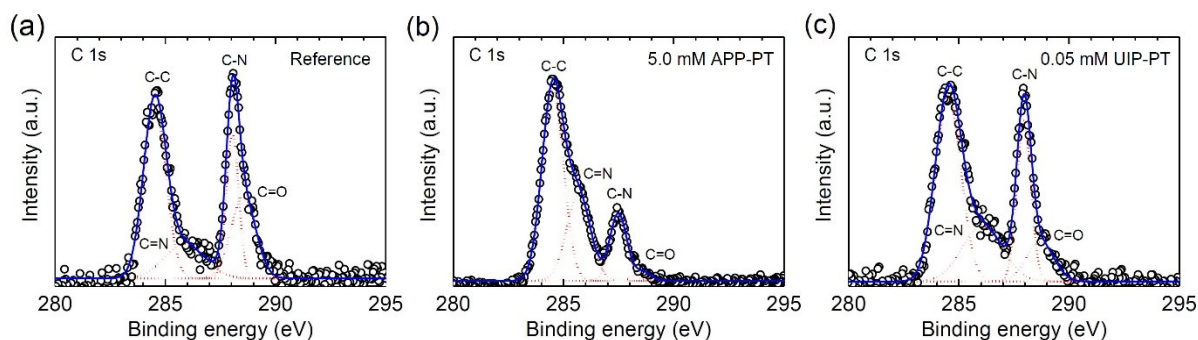
Figure S4. C 1s XPS spectra for (a) the reference, (b) 5.0 mM APP-PT and (c) 0.05 mM UIP-PT samples. The binding energy of 284.6 eV was assigned to the C-C bond, which was used for calibration of binding energy.
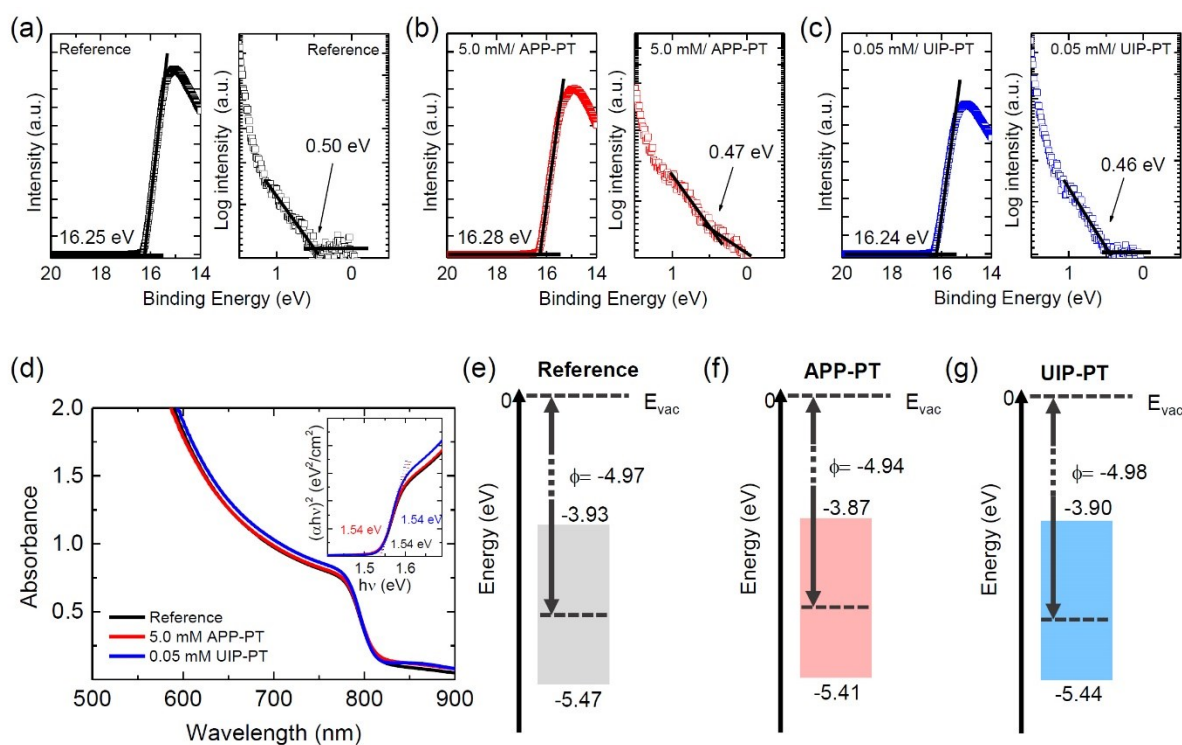

Figure S5. UPS (He 1a, E=21.22 eV) spectra showing the cut-off (left panel) and the Fermi edge onset (right panel) region for (a) the reference, (b) APP-PT and (c) UIP-PT films. The perovskite films were prepared on Si wafer substrates. (d) Visible spectra of the perovskite films before and after APP-PT or UIP-PT. Inset shows Tauc plot. (e)-(g) Schematic energy levels constructed by the UPS and Tauc plot results.
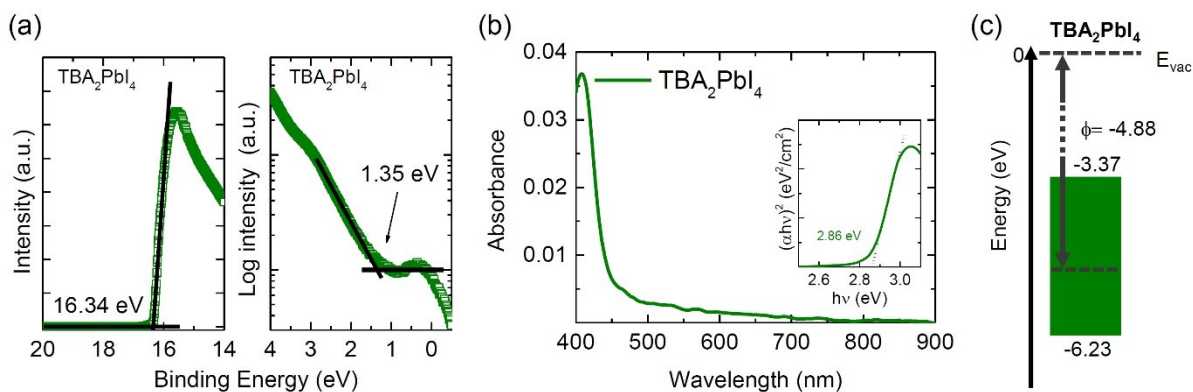
Figure S6. (a) UPS spectra showing the cut-off (left panel) and the Fermi edge onset (right panel) region for the TBA_2PbI_4 film. (b) UV-Visible spectra of the TBA_2PbI_4 films with a Tauc plot in inset Figure. (c) Schematic energy levels constructed by the UPS and optical bandgap from the Tauc plot.
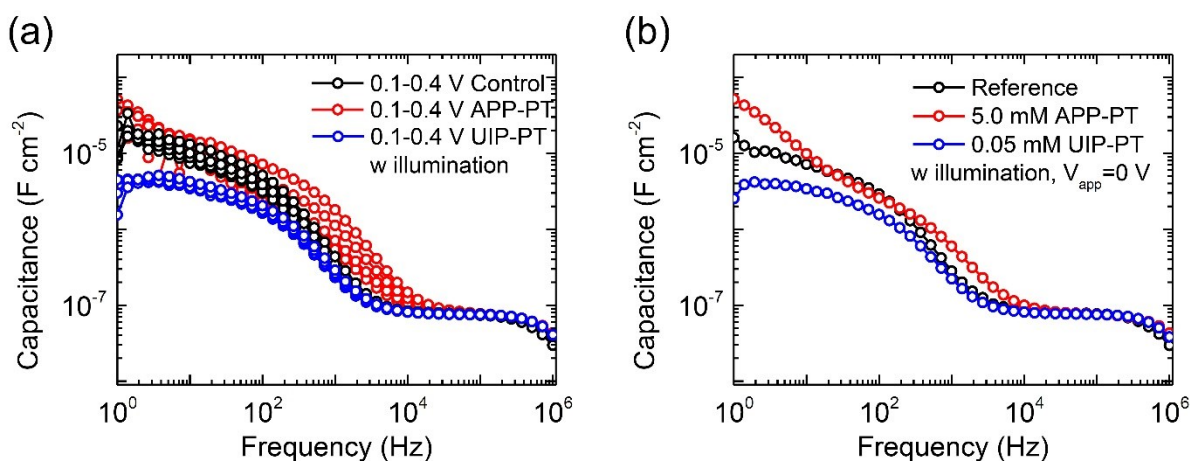

Figure S7. Capacitance-frequency curves measured under one sun condition with applied voltage (a) from 0.1 to 0.4 V (0.1 V step size) and (b) short circuit condition (applied voltage is 0 V) with the device structure of FTO/perovskite/Au.

Table S1. Capacitance at low frequency region ($f = 1.0$ Hz), geometrical capacitance (C_g) extracted from high frequency region ($f = 10^5$ Hz) and dielectric constant (k) measured from FAPbI$_3$ films without and with post-treatment based on APP-PT and UIP-PT. The dielectric constants (k) were calculated using an equation given by $C_g = k\varepsilon_0 \times A/L$ where ε_0 is the vacuum permittivity, A is the active area of 0.294 cm^2, and L is the film thickness of 520 nm [1, 2].

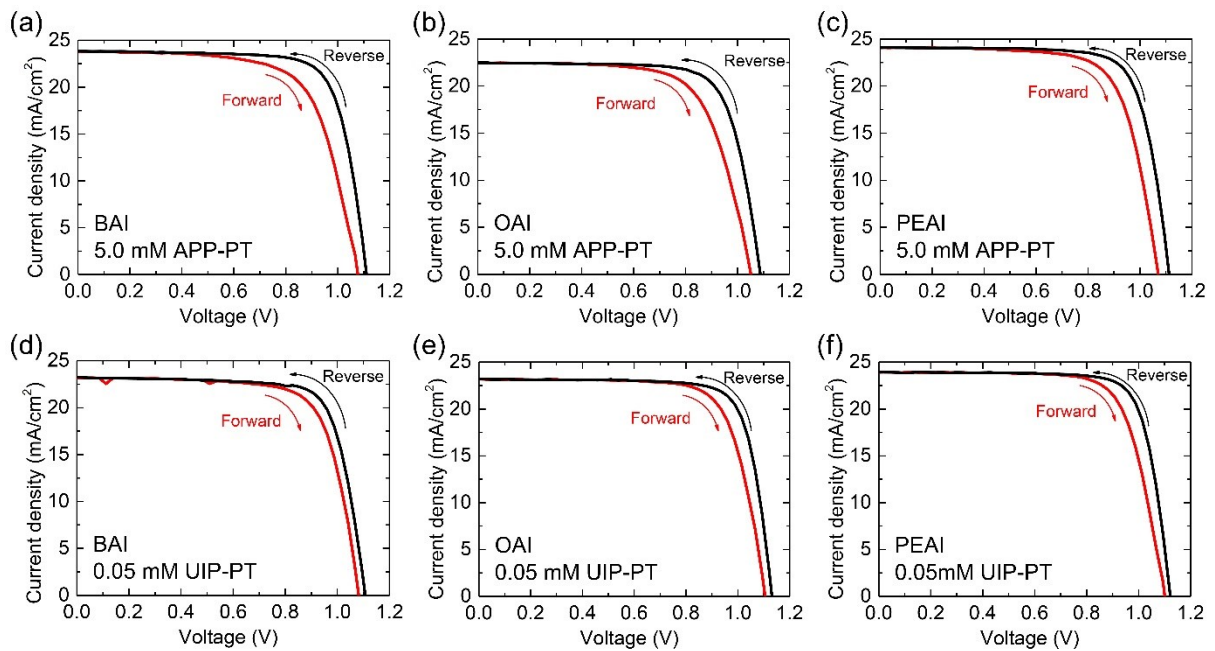|	Capacitance at $f = 1.0$ Hz (F/cm^2)	Geometrical capacitance (F/cm^2)	Dielectric constant
Reference	1.60×10^{-5}	7.66×10^{-8}	45.01
5.0 mM APP-PT	5.15×10^{-5}	7.52×10^{-8}	44.21
0.05 mM UIP-PT	2.53×10^{-6}	7.56×10^{-8}	44.40

Figure S8. J-V curves of the best performing PSCs with post-treatment based on (a-c) APP-PT and (d-f) UIP-PT with BAI, OAI and PEAI as passivating agents, measured under AM 1.5 G one sun illumination (100 mW/cm^2) at a scan rate of 130 mV/s. The aperture area was 0.125 cm^2.

Table S2. Power conversion efficiency (PCE) and hysteresis index (HI) for the best performing PSCs employing FAPbI$_3$ perovskite layers with post-treatment based on APP-PT and UIP-PT using BAI, OAI and PEAI. RS and FS stands for reverse scan and fowrard scan, respectively.

Post-treatment	Scan direction Hysteresis index (HI)	PCE (%) BAI	PCE (%) OAI	PCE (%) PEAI
APP-PT	RS	20.12	20.17	20.47
	FS	17.47	18.11	18.58
	HI	0.032	0.035	0.037
UIP-PT	RS	19.57	20.54	21.02
	FS	18.32	19.02	19.45
	HI	0.024	0.024	0.019

References

[1] O. Almora, C. Aranda, E. Mas-Marza and G. Garcia-Belmonte, *Appl. Phys. Lett.*, 2016, **109**, 173903.

[2] J. Chen and N.-G. Park, *Adv. Mater.*, 2019, **31**, 1803019.