

Supplementary Materials

Pyridine derivatives desorb physisorbed multilayers from dip-coated self-assembled monolayers for scalable and efficient perovskite solar cells

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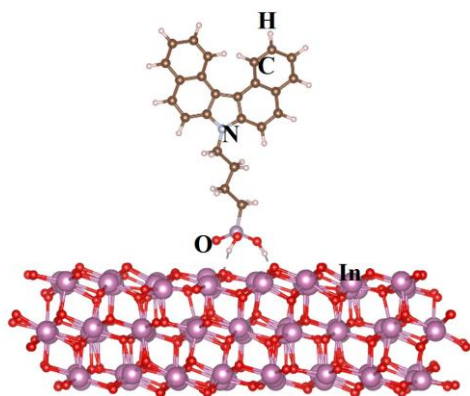
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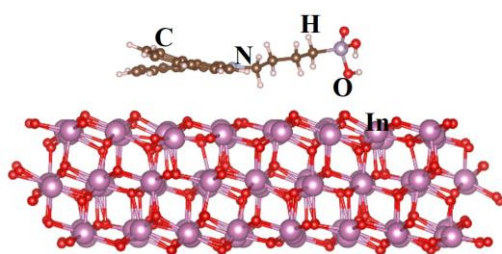
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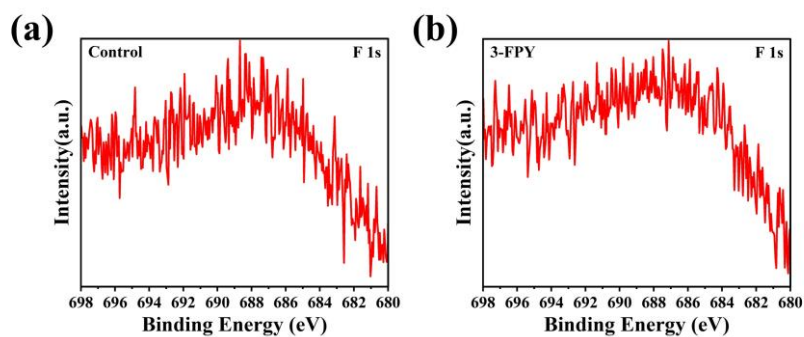
hydrogen bonding

Supplementary Figure 1. The hydrogen bonding adsorption configurations via the phosphonic acid -OH group.

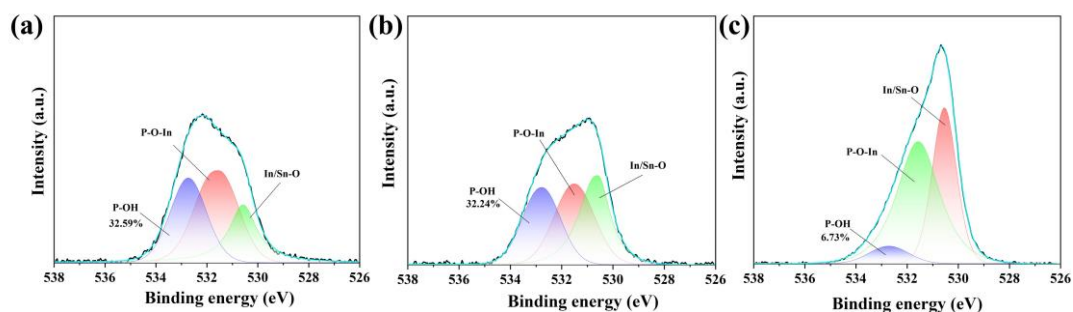


carbazole

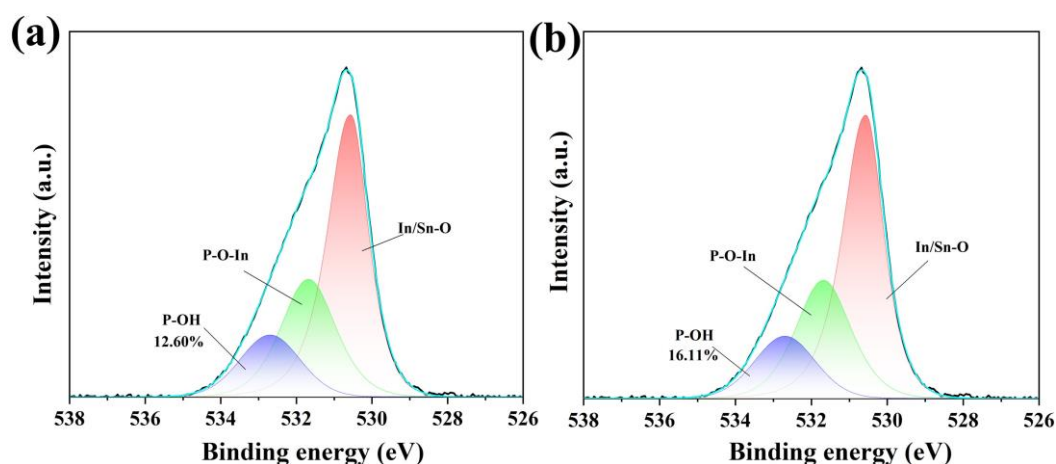
Supplementary Figure 2. The adsorption configurations of weaker interactions through the terminal carbazole moiety.



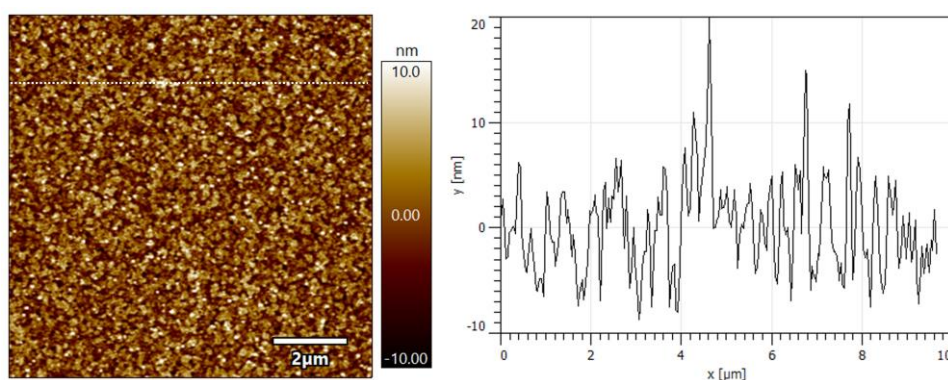
Supplementary Figure 3. The F 1s XPS spectra of different SAM substrate, (a) for control, and (b) for 3-FPy post treatment.



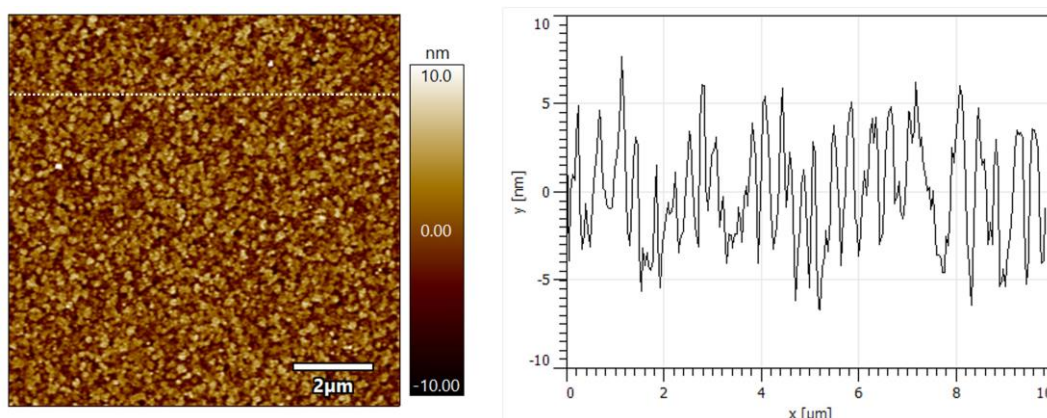
Supplementary Figure 4. O 1s XPS spectra of SAM-coated ITO substrates: (a) dip-coated, as-prepared; (b) dip-coated, annealed; (c) pyridine-flushed, without annealing.



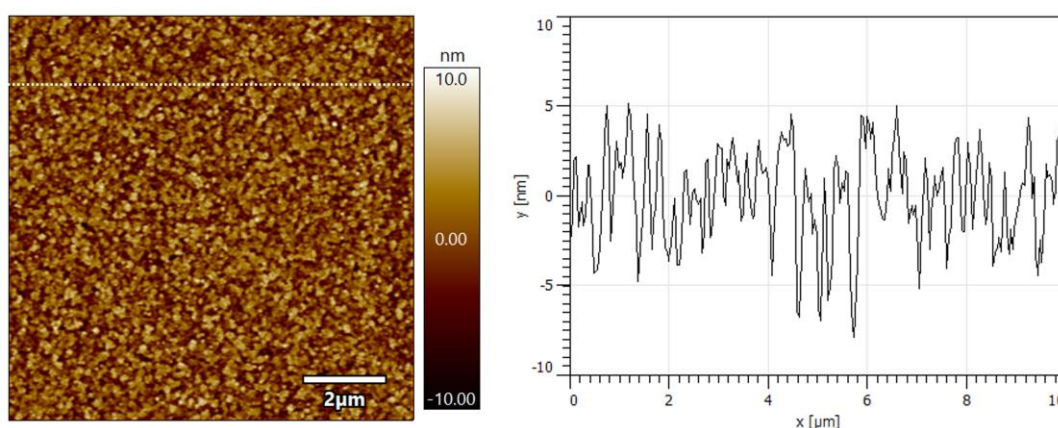
Supplementary Figure 5. The O 1s XPS spectra of SAM dip-coated substrate with different solvents post-treatment. (a) for IPA post-treatment, (b) for DMSO post-treatment.



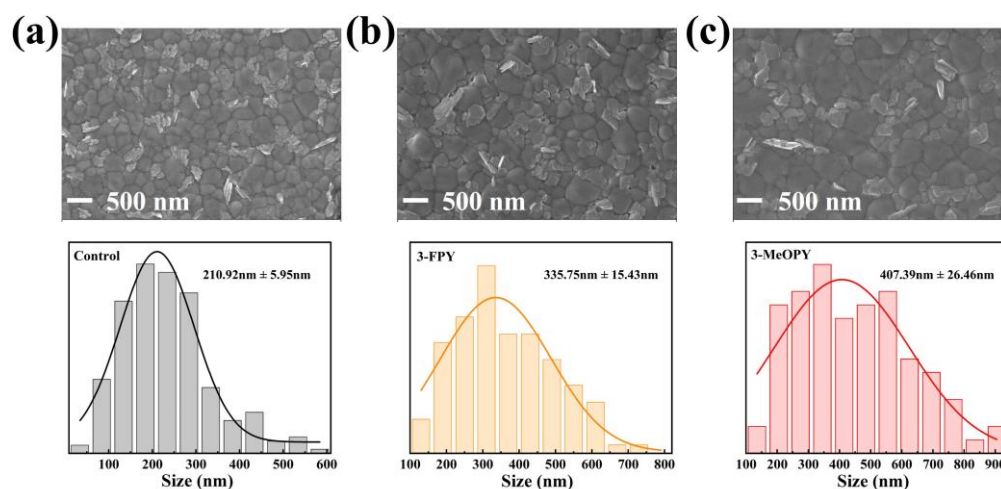
Supplementary Figure 6. Topographical AFM images of control SAM substrate and corresponding section analysis.



Supplementary Figure 7. Topographical AFM images of 3-FPy post-treatment SAM substrate and corresponding section analysis.

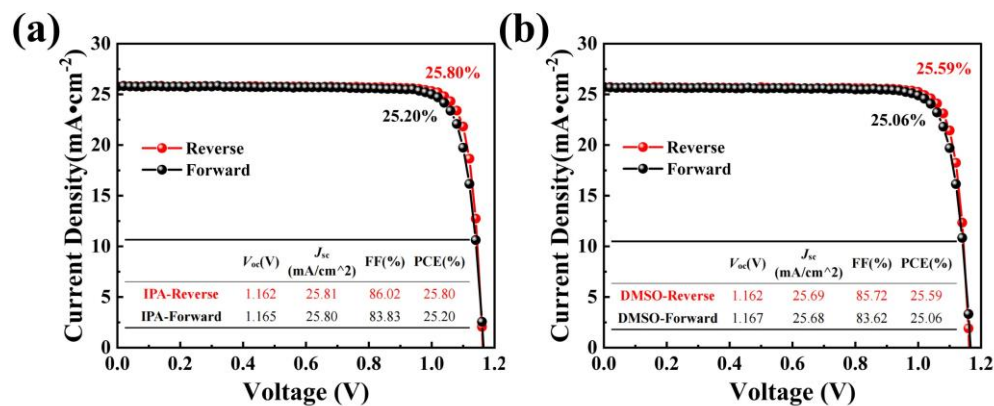


Supplementary Figure 8. Topographical AFM images of 3-MeOPy post-treatment SAM substrate and corresponding section analysis.

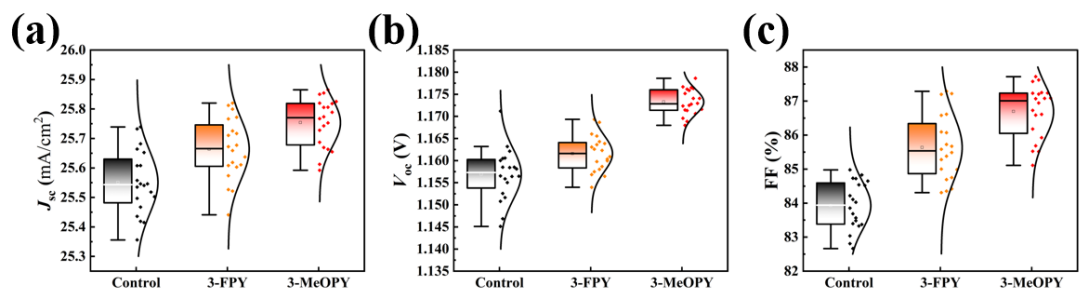


Supplementary Figure 9. Grain size distribution histogram derived from the SEM images of perovskite film prepared on (a) control, (b) 3-FPy and (c) 3-MeOPy post

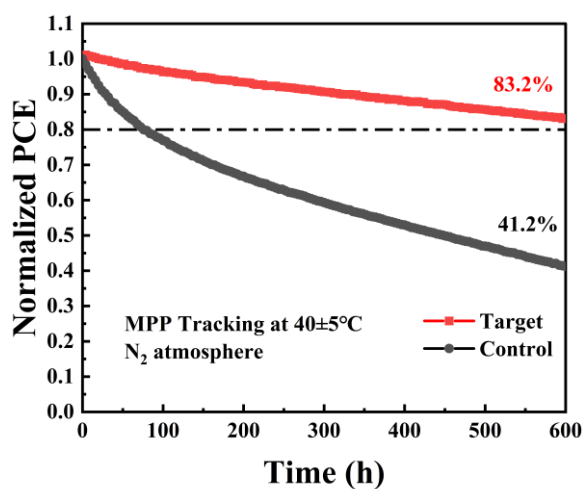
treatment SAM substrate.



Supplementary Figure 10. The J - V curves of the champion devices for IPA and DMSO-treated SAMs, (a) for IPA treated and (b) for DMSO treated.



Supplementary Figure 11. Statistical data of photovoltaic parameters extracted from the current density-voltage (J - V) characteristics of devices fabricated based on control and target SAM, based on 20 independent devices for each condition. (a) Short-circuit current density (J_{sc}). (b) Open-circuit voltage (V_{oc}). (c) Fill factor (FF). The center line, box, and whiskers represent the median, interquartile range (25th-75th percentiles), and data within $1.5\times$ the interquartile range, respectively.



Supplementary Figure 12. Maximum power point (MPP) tracking of the unencapsulated devices in an N₂ atmosphere under one-sun white-light LED illumination.

Supplementary Table 1. The fitting results of TRPL curves for control and target perovskite films

Condition	A ₁ (%)	τ ₁ (ns)	A ₂ (%)	τ ₂ (ns)	τ _{avg} (ns)
Control	21.08	203.26	78.92	1,690.97	1,644.23
3-FPy	27	163.15	73	1,855.28	1,712.48
3-MeOPy	28.65	153.27	71.35	1,887.81	1,702.44

The TRPL decay curves were fitted using a biexponential function with a constant offset, according to the following equation:^[1,2]

$$Y = A_1 \exp(-\frac{t}{\tau_1}) + A_2 \exp(-\frac{t}{\tau_2}) + y_0$$

where A_1 and A_2 are the amplitudes of the fast and slow decay components, τ_1 and τ_2 are the corresponding lifetimes, and y_0 is a constant offset accounting for the background signal. The average lifetime (τ_{avg}) was calculated using the equation below: ^[3,4]

$$\tau_{avg} = (A_1\tau_1^2 + A_2\tau_2^2)/(A_1\tau_1 + A_2\tau_2)$$

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