

Supporting Information

Inhibiting defect formation and degradation at the buried interface of tin perovskite solar cells by modulating PEDOT:PSS with sodium alginate

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Experimental section

Materials: Formamidinium iodide (FAI, 99.9%), methylammonium iodide (MAI, 99.9%), ethylenediamine diiodide (EDA₂, 99.5%), BCP (99.9%) and lead iodide (PbI₂, 99.99%) were purchased from Xi'an Yuri Solar Co., Ltd. PEDOT:PSS (AI 4083) was acquired from Heraeus Materials Technology Co., Ltd. Chlorobenzene (CB, 99.50%), N,N-dimethylformamide (DMF, 99.80%), dimethyl sulfoxide (DMSO, 99.90%), tin (II) iodide (SnI₂, 99.99%), Cesium iodide (CsI, 99.9%), tin(II) fluoride (SnF₂, 99%), and 2-Propanol (IPA, 99.999%) were purchased from Sigma-Aldrich. Guanidine hydroiodide (GAI, 98%) was purchased from J&K Scientific. Glycine hydrochloride (GlyHCl, 99%) was purchased from Shanghai Macklin Biochemical Co., Ltd. Pyrophosphoric acid (PP, 95%) was purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. All chemicals were used as received without further purification.

Device Fabrication: The ITO substrates were sequentially ultrasonicated in deionized water, acetone, and ethanol for 15 min each, dried with high-purity N₂, and then treated with UV-ozone for 20 min. Then, the PEDOT:PSS solution was spin-coated onto the substrates at 3500 rpm for 30 s and annealed at 120 °C for 20 min, followed by spin-coating a 1.0 mg/mL SA solution at 3500 rpm for 30 s and annealing at 100 °C for 5 min. The samples were then transferred to a glovebox for perovskite deposition. The SA solution was prepared by dissolving 1.0 mg of SA powder in 1 mL of H₂O to obtain a 1.0 mg/mL solution. A precursor solution containing 128.98 mg FAI, 39.74 mg MAI, 372.52 mg SnI₂, 0.01870 mg GAI, and 15.67 mg SnF₂ in a mixture of DMF (800 μL) and DMSO (200 μL) was spin-coated at 6000 rpm for 60 s to form FA_{0.75}MA_{0.25}SnI₃

films. At the 12th second, 180 μL of CB was dripped onto the film, followed by a 100 $^{\circ}\text{C}$ annealing for 10 min. A precursor solution containing 185.7 mg FAI, 85.8 mg MAI, 335.3 mg SnI_2 , 414.9 mg PbI_2 , 4 mg GlyHCl, and 14.1 mg SnF_2 in a mixture of DMF (750 μL) and DMSO (250 μL) was spin-coated at 5000 rpm for 50 s to form $\text{Cs}_{0.1}\text{FA}_{0.6}\text{MA}_{0.3}\text{Pb}_{0.5}\text{Sn}_{0.5}\text{I}_3$ films. At the 25th second, 200 μL of CB was dripped onto the film, followed by a 100 $^{\circ}\text{C}$ annealing for 10 min. PP (0.5 mg/mL) and EDAI_2 (0.5 mg/mL) were sequentially spin-coated onto the $\text{Cs}_{0.1}\text{FA}_{0.6}\text{MA}_{0.3}\text{Pb}_{0.5}\text{Sn}_{0.5}\text{I}_3$ films at 3000 rpm for 20 s, followed by annealing at 100 $^{\circ}\text{C}$ for 5 min separately. Finally, 35 nm C_{60} , 7 nm BCP, and 80 nm Ag were thermally evaporated sequentially onto the perovskite layer under a vacuum of 5×10^{-4} Pa through a shadow mask to complete the perovskite solar cells.

Characterization: The *J-V* characteristics were carried out using Keithley 2400 under AM 1.5 G illumination (100 mW cm^{-2}) from a solar simulator (Oriel Sol3A Class Solar Simulator). The IPCE curves were measured by a QTest Station 500AD Solar Cell Quantum Efficiency System (CROWNTECH, INC.). The SEM images were obtained by using a Hitachi S-4800 field-emission scanning electron microscopy. The instrument for testing AFM images were icon/Dimension icon from Bruker Instrument Co. Ltd. X-ray diffraction patterns were examined by a Bruker D8 ADVANCE XRD equipment. Absorption spectra were obtained by Shimadzu UV-vis 3600 spectrophotometer (UV-3600). PL spectra were measured with a pulse laser at 510 nm (EI, FLS920). EIS were studied by the Zahner electrochemical workstation under dark condition. XPS and UPS spectra were recorded by PHI Quantera SXM (ULVAC-PHI).

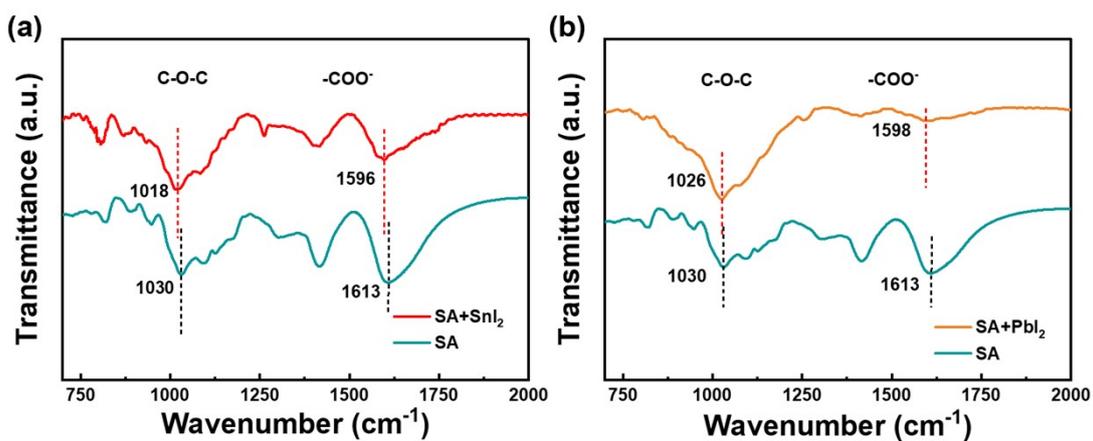


Figure S1. The FTIR spectra of SA and the mixture of SA with (a) SnI₂ and (b) PbI₂.

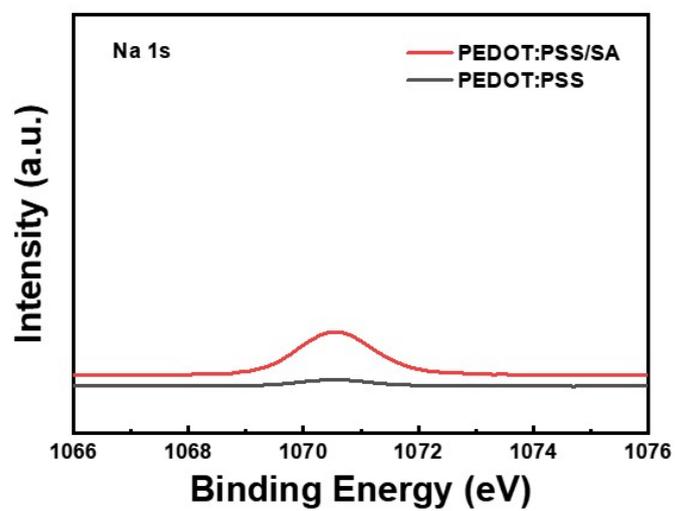


Figure S2. Na 1s XPS spectra of PEDOT:PSS and PEDOT:PSS/SA films.

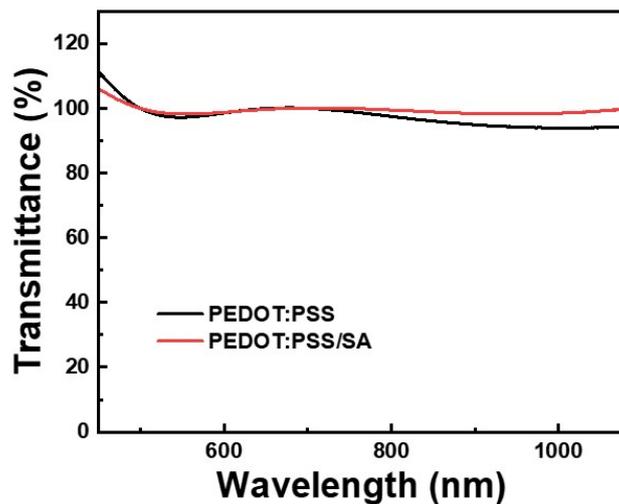


Figure S3. Transmittance of PEDOT:PSS films without and with SA modification.

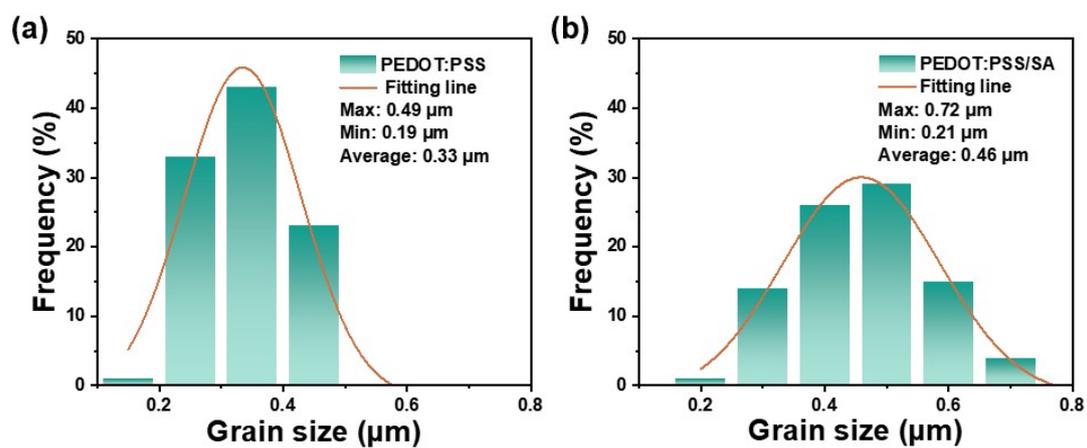


Figure S4. Grain size distribution of Sn perovskite deposited on (a) PEDOT: PSS and (b) SA-modified PEDOT: PSS films.

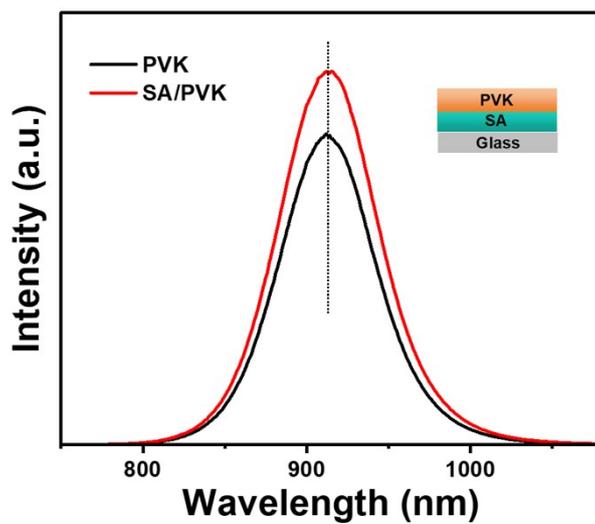


Figure S5. Steady-state PL spectra of perovskite films prepared on bare glass and glass/SA substrates.

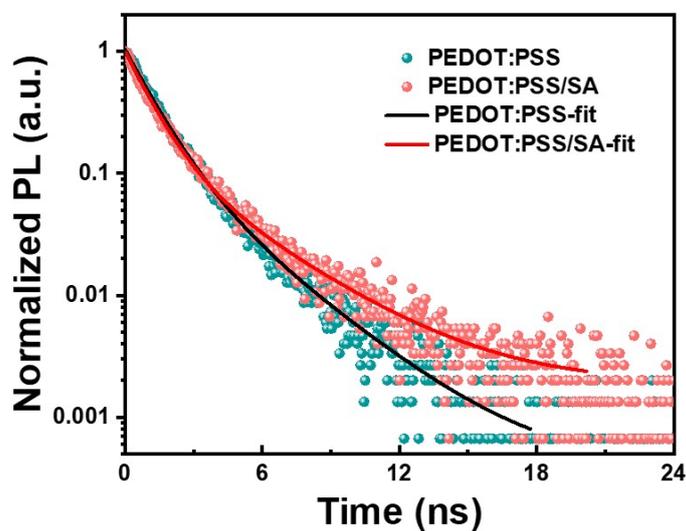


Figure S6. TRPL spectra of perovskite films based on the control and SA-modified PEDOT:PSS.

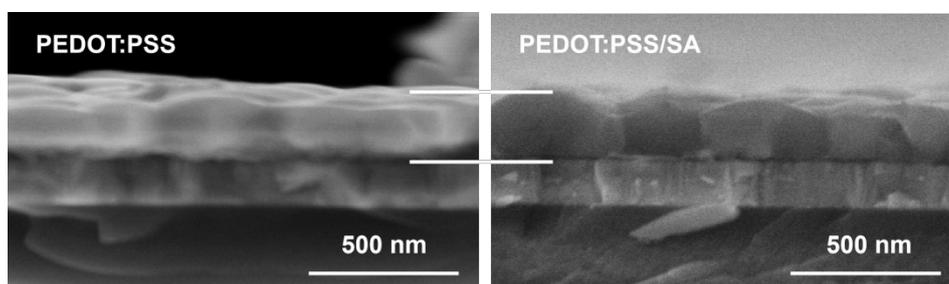


Figure S7. Cross-sectional SEM images of perovskite films deposited on PEDOT:PSS and SA-modified PEDOT:PSS.

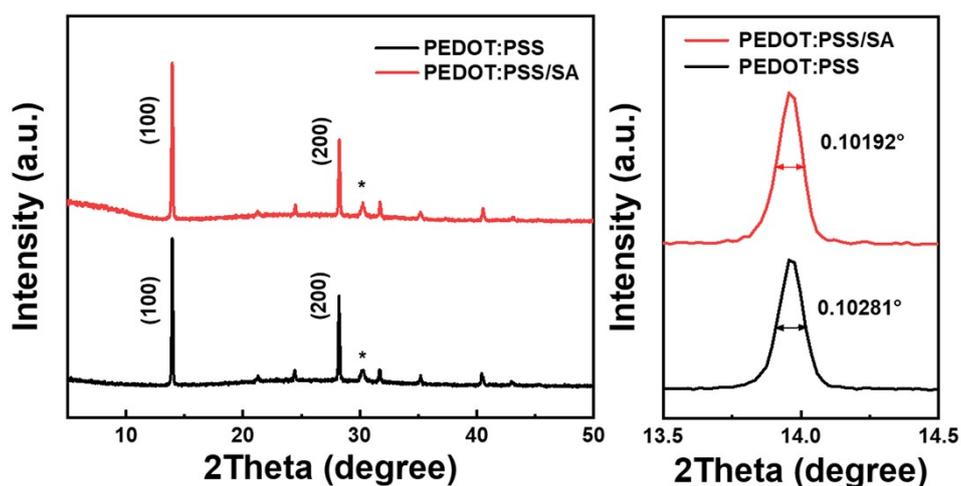


Figure S8. XRD patterns of Sn perovskite films and the corresponding FWHM values of (100) peak.

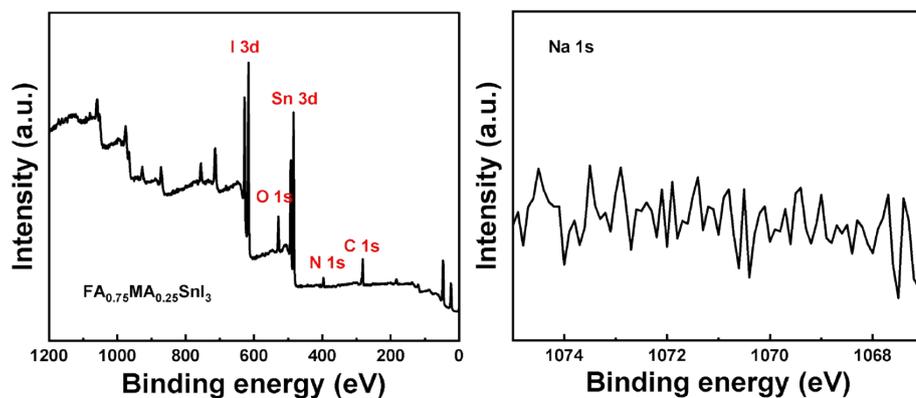


Figure S9. XPS spectra for the perovskite film deposited on PEDOT:PSS/SA and the Na 1s spectra.

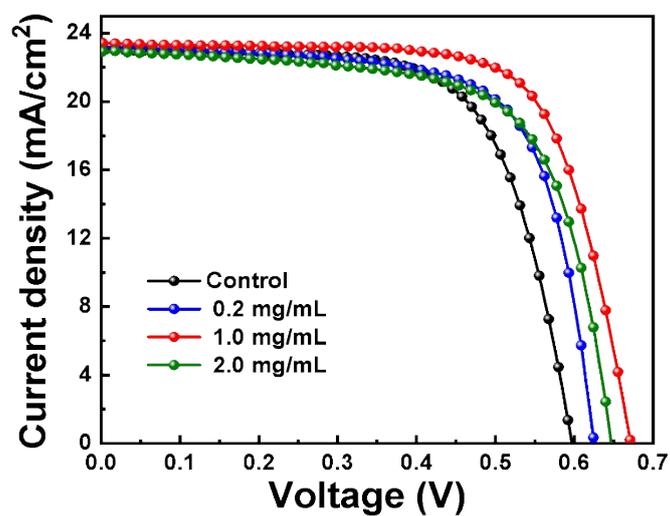


Figure S10. *J-V* curves of TPSCs fabricated on PEDOT:PSS modified with different concentrations of SA.

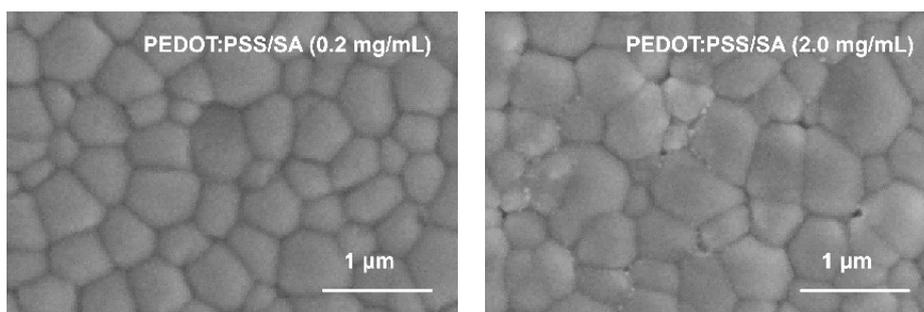


Figure S11. SEM images of perovskite films prepared on PEDOT:PSS modified with different concentrations of SA.

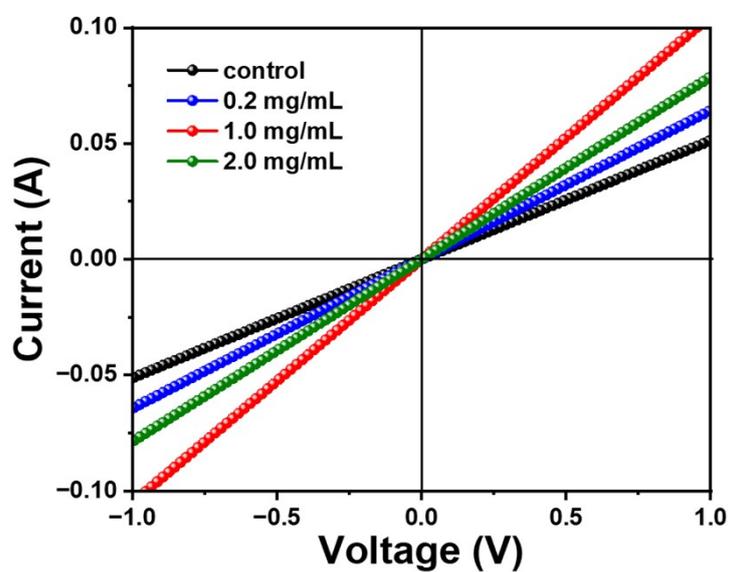


Figure S12. Current-voltage curves of PEDOT:PSS films modified with different concentrations of SA.

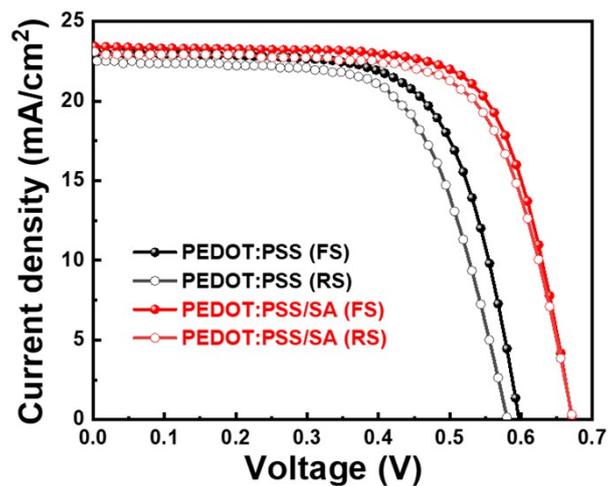


Figure S13. *J-V* curves of PSCs measured under the reverse and forward scanning directions.

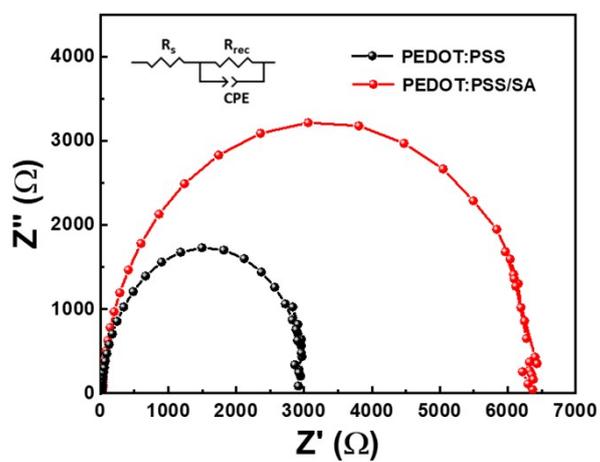


Figure S14. Nyquist plots of the control and SA-modified devices.

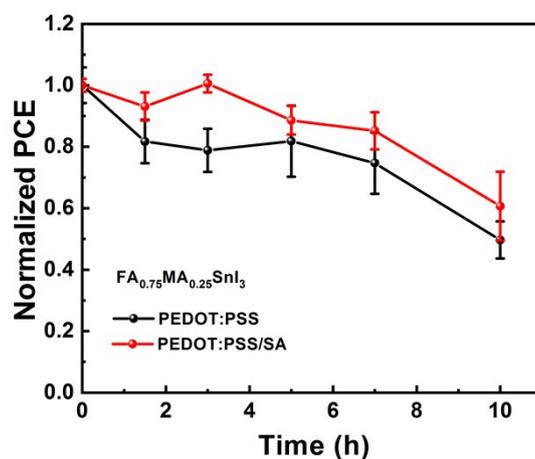


Figure S15. The stability of unsealed devices stored in air.

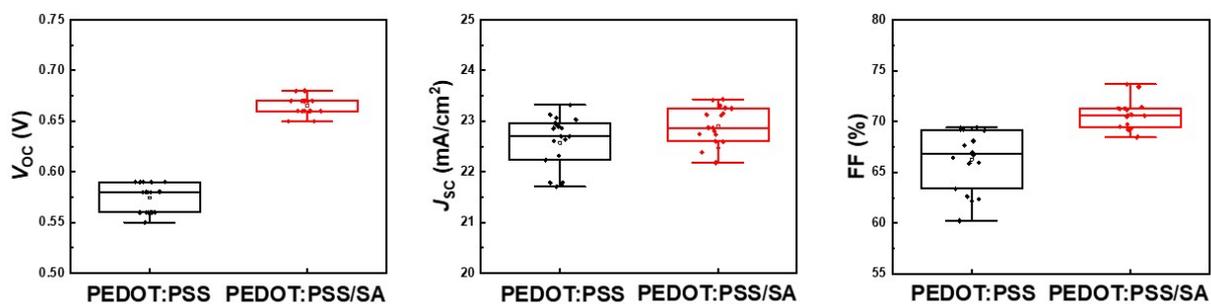


Figure S16. The statistical evaluation of PCE, V_{OC} , J_{SC} , and FF of TPSCs with pristine PEDOT:PSS and the SA modified PEDOT:PSS films.

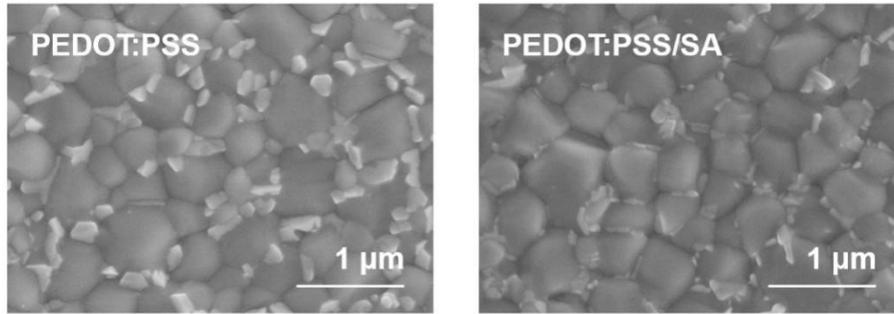


Figure S17. SEM images of perovskite films for $\text{Cs}_{0.1}\text{FA}_{0.6}\text{MA}_{0.3}\text{Sn}_{0.5}\text{Pb}_{0.5}\text{I}_3$ -based PSCs on PEDOT:PSS and PEDOT:PSS/SA films.

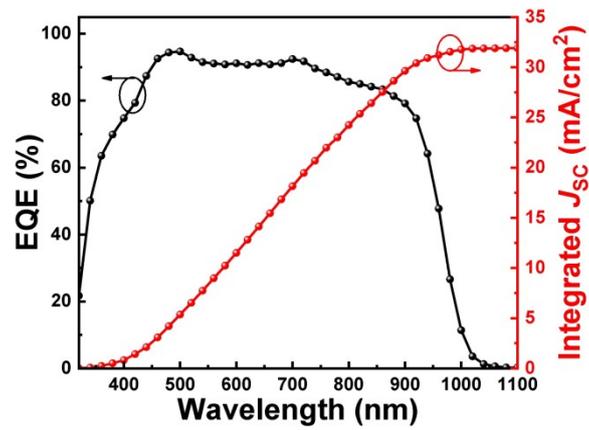


Figure S18. EQE spectra and the corresponding integrated J_{sc} for $\text{Cs}_{0.1}\text{FA}_{0.6}\text{MA}_{0.3}\text{Sn}_{0.5}\text{Pb}_{0.5}\text{I}_3$ -based PSCs.

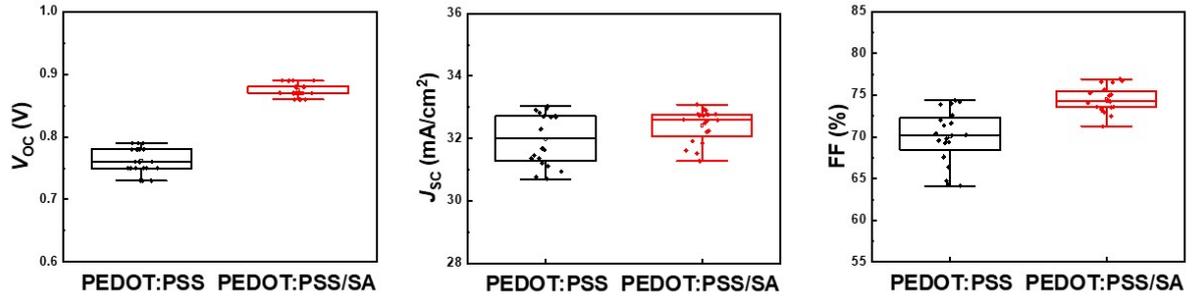


Figure S19. The statistical evaluation of PCE, V_{OC} , J_{SC} , and FF of Sn-Pb PSCs with pristine PEDOT:PSS and the modified-PEDOT:PSS films with SA.

Table S1. Fitted PL lifetimes for perovskite films deposited on the control and SA modified PEDOT:PSS. The average carrier lifetime (τ_{ave}) was calculated by $\tau_{ave} = A_1\tau_1 + A_2\tau_2$.

Sample	A_1	τ_1 (ns)	A_2	τ_2 (ns)	τ_{ave} (ns)
PEDOT:PSS	0.85	1.13	0.15	2.95	1.40
PEDOT:PSS/S A	0.84	1.04	0.16	3.48	1.43

Table S2. Performance parameters of $FA_{0.75}MA_{0.25}SnI_3$ TPSCs fabricated from PEDOT:PSS films modified with SA at different concentrations.

Device (mg/mL)	V_{OC} (V)	J_{SC} (mA/cm ²)	FF (%)	PCE (%)
Control	0.59	23.03	68.11	9.29
0.2	0.62	23.19	69.54	10.07
1.0	0.67	23.43	71.22	11.20
2.0	0.64	22.94	68.15	10.00

Table S3. PV parameters of the control and target devices. The hysteresis index (HI) is calculated using the following formula: $HI = (PCE_{FS} - PCE_{RS}) / PCE_{FS}$

Device	Scan direction	V_{OC} (V)	J_{SC} (mA/cm ²)	FF (%)	PCE (%)	HI
PEDOT:PSS	FS	0.59	23.03	68.11	9.29	0.08
	RS	0.58	22.50	65.44	8.54	
PEDOT:PSS/S A	FS	0.67	23.43	71.22	11.20	0.04
	RS	0.67	23.09	69.29	10.72	

