

Supporting Information for

Effect of Hammett substituent constant of *para*-substituted benzoic acid on the perovskite/SnO₂ interface passivation in perovskite solar cells

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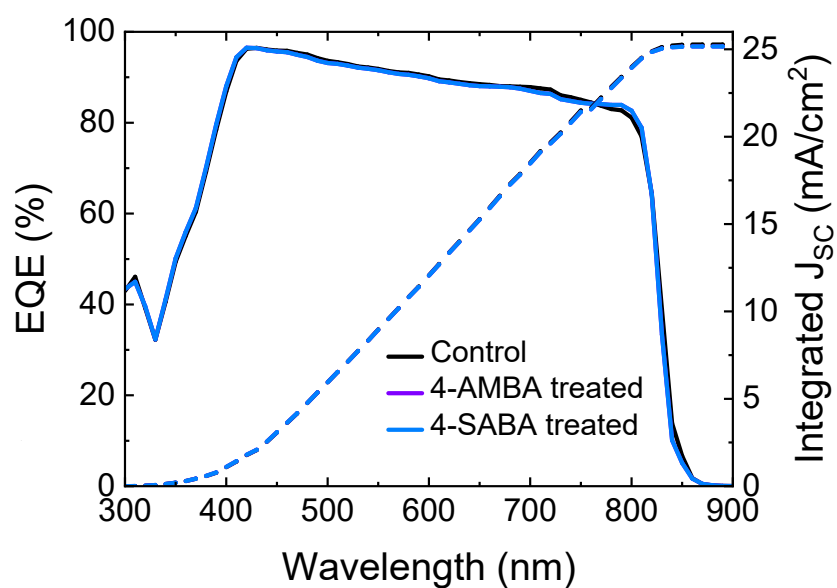


Figure S1. EQE spectra with the integrated J_{SC} for PSCs with the bare SnO_2 (control), 4-AMBA- and 4-SABA-treated SnO_2 .

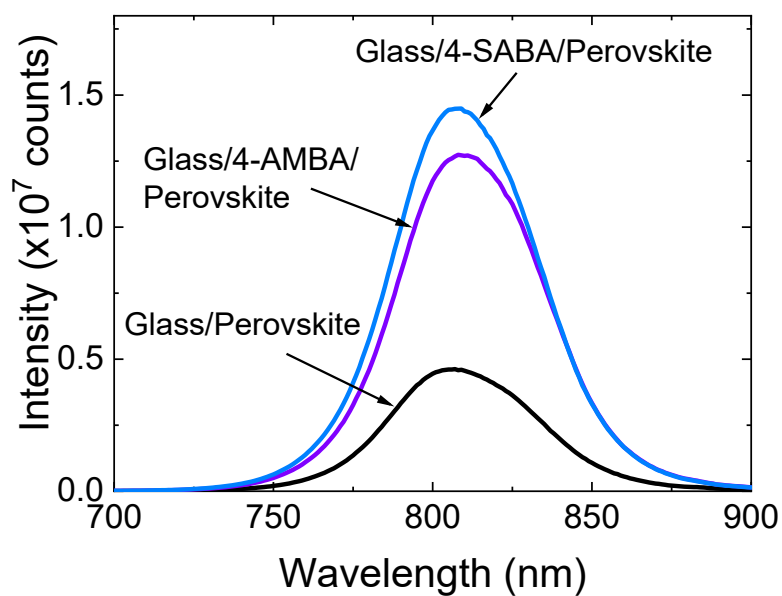


Figure S2. SSPL of the perovskite films deposited on glass without and with 4-AMBA and 4-SABA treatment.

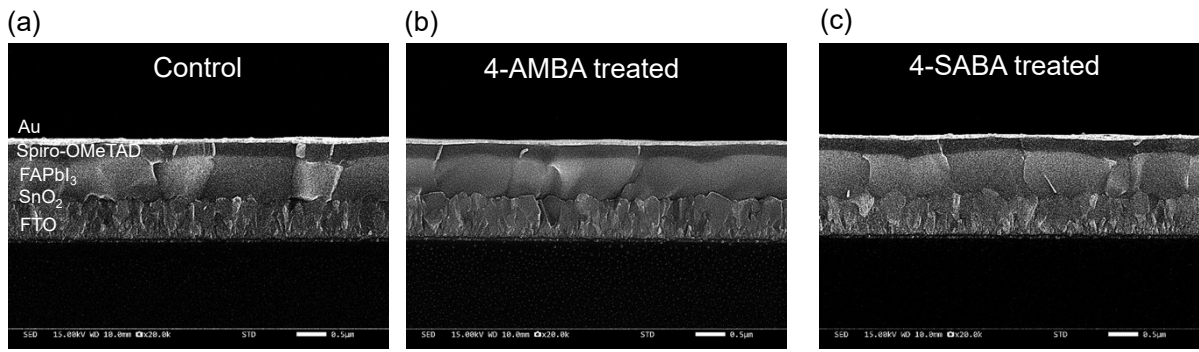


Figure S3. Cross-sectional SEM images of full device. (a) FTO/SnO₂/perovskite/Spiro-OMeTAD/Au. (b) FTO/SnO₂/4-AMBA/perovskite/Spiro-OMeTAD/Au. (c) FTO/SnO₂/4-SABA/perovskite/Spiro-OMeTAD/Au.

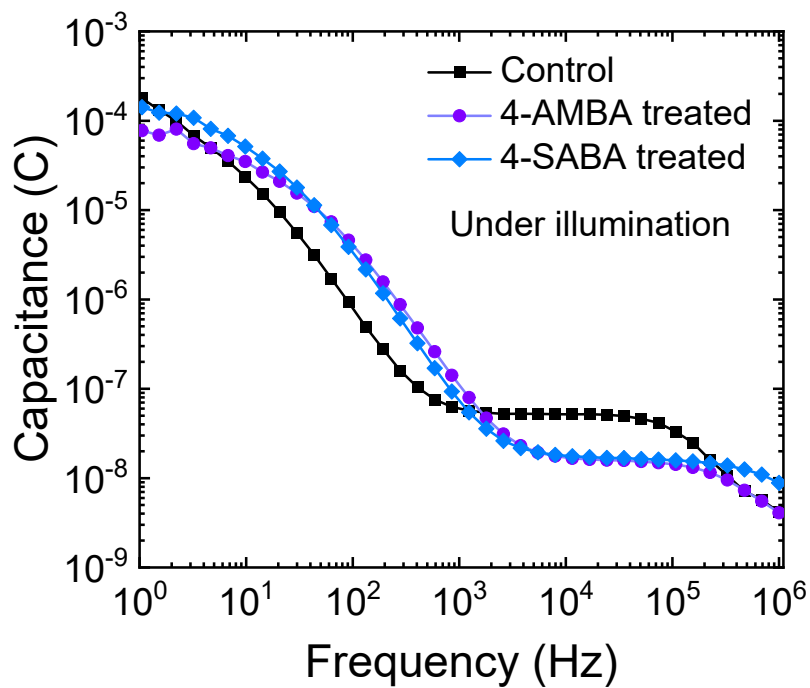


Figure S4. Capacitance frequency (C-f) plots of PSCs based on SnO₂, 4-AMBA-treated SnO₂ and 4-SABA-treated SnO₂.

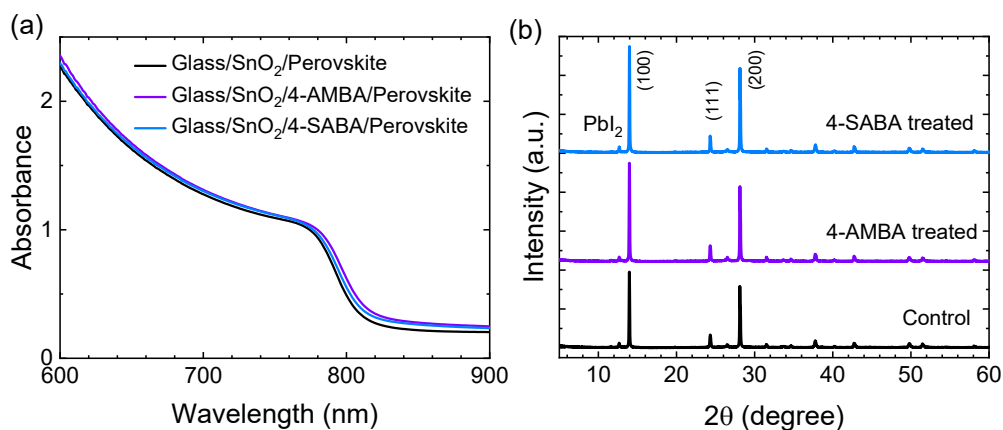


Figure S5. (a) UV-vis absorption spectra and (b) XRD patterns of perovskite coated on SnO₂, 4-AMBA modified SnO₂, and 4-SABA modified SnO₂.

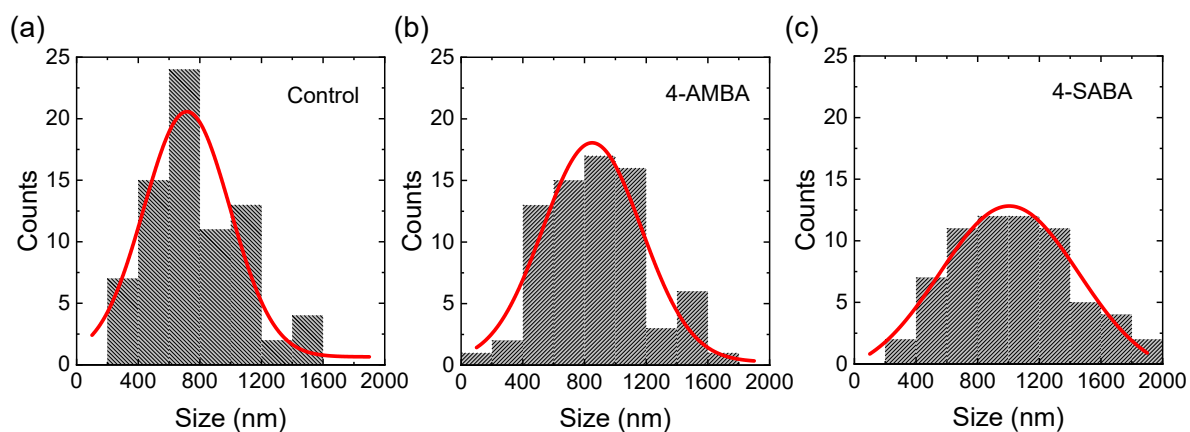


Figure S6. Perovskite grain size distribution estimated from the surface SEM image for (a) control, (b) 4-AMBA treated and (c) 4-SABA treated samples.

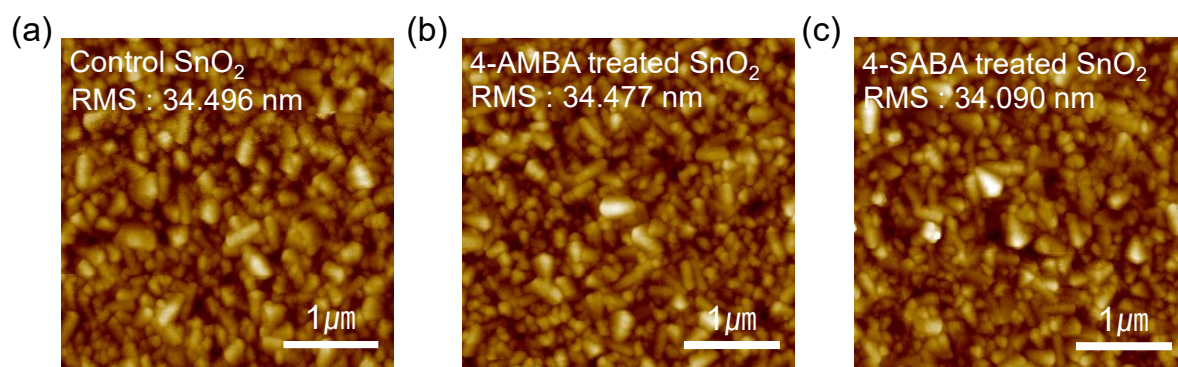


Figure S7. AFM images of (a) the bare SnO₂, (b) the 4-AMBA treated SnO₂ and (c) the 4-SABA treated SnO₂.

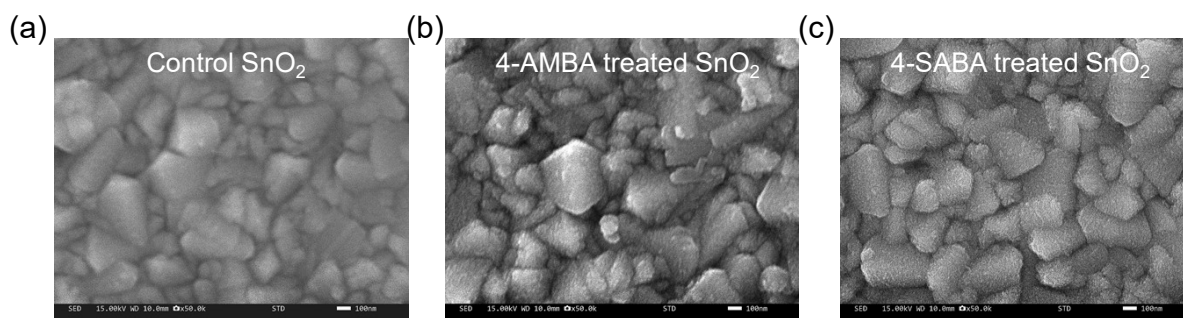


Figure S8. Top-view SEM images of (a) the bare SnO₂ (b) the 4-AMBA treated SnO₂ and (c) the 4-SABA treated SnO₂. SnO₂ was deposited on FTO.

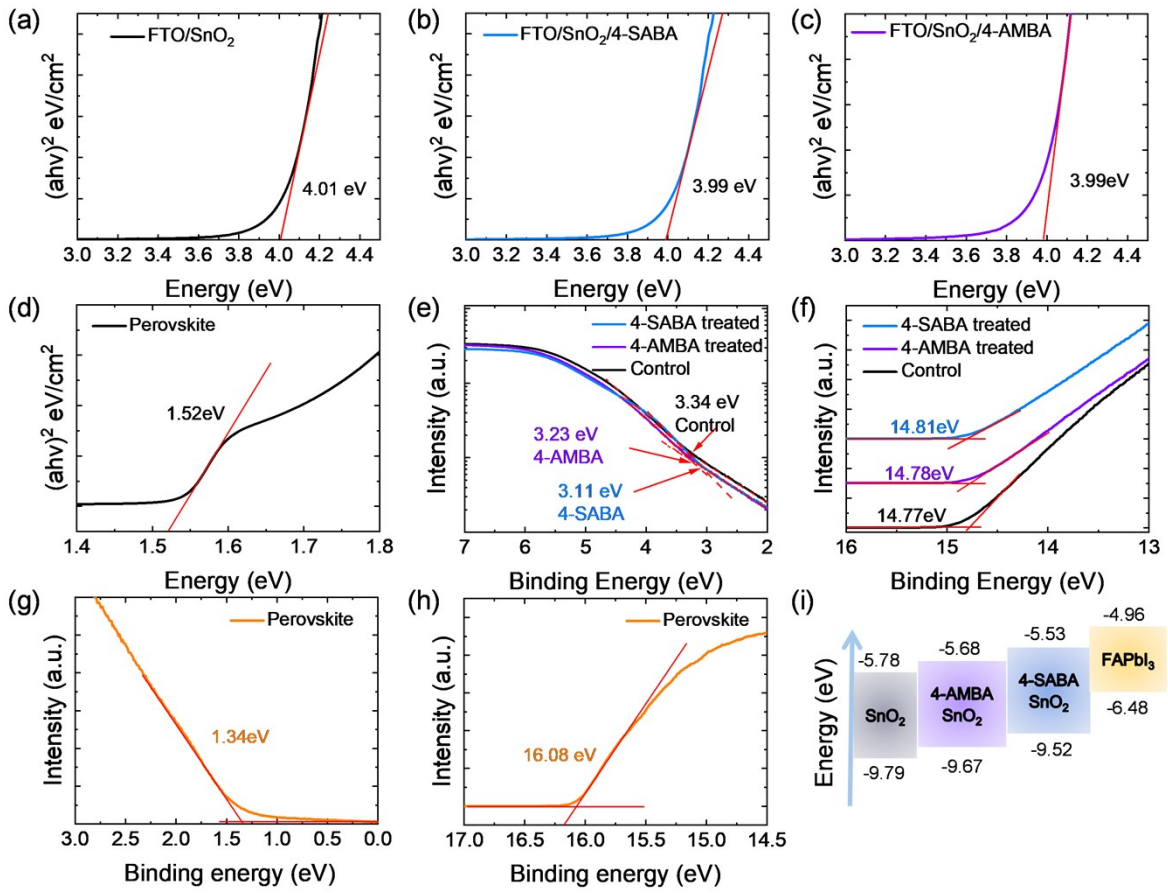


Figure S9. Tauc plots for (a) SnO₂ (b) 4-AMBA treated SnO₂ (c) 4-SABA treated SnO₂ and (d) perovskite film. UPS spectra of (e) Fermi edge energy and (f) cut-off energy for SnO₂, 4-AMBA treated SnO₂ and 4-SABA treated SnO₂. (g) Fermi edge energy and (h) cut-off energy for perovskite. (i) Schematic illustration of energy level of SnO₂, 4-AMBA treated SnO₂, 4-SABA treated SnO₂ and perovskite.

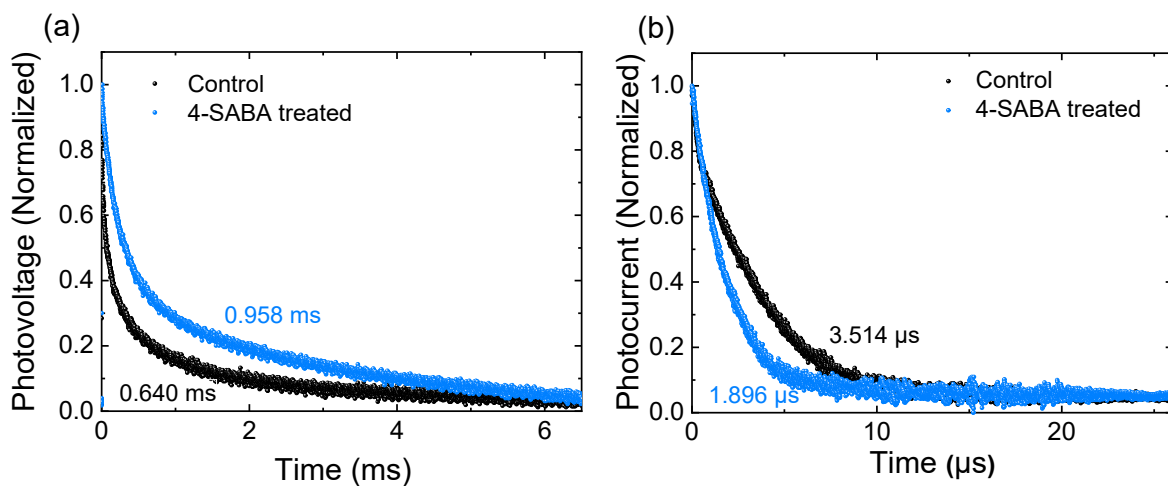


Figure S10. (a) TPV and (b) TPC data of device on FTO/SnO₂/Perovskite/Spiro-OMeTAD/Ag and FTO/SnO₂/4-SABA/Perovskite/Spiro-OMeTAD/Ag.

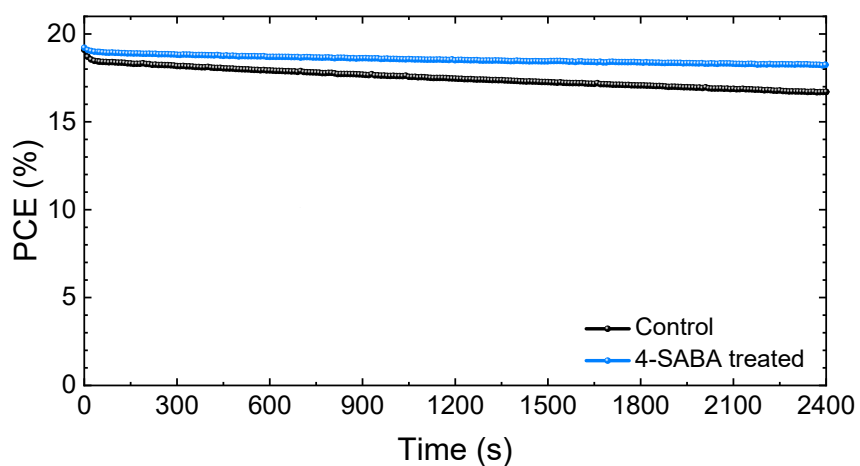


Figure S11. SPO of the unencapsulated PSCs employing unmodified and 4-SABA treated SnO₂ obtained by maximum power point tracking under 1 sun.

Table S1. Calculated parameters of geometric capacitance (C), trap-filled limited voltage (V_{TFL}), dielectric constant (ϵ) and trap density (n_t).

Sample	C (F)	V_{TFL} (V)	ϵ	Area (cm ²)	n_t (cm ⁻³)
SnO ₂	5.1796×10^{-8}	1.068	147.92	0.28	3.48×10^{16}
SnO ₂ /4-AMBA	1.6902×10^{-8}	1.028	48.27	0.28	1.09×10^{16}
SnO ₂ /4-SABA	1.7703×10^{-8}	0.926	50.56	0.28	1.03×10^{16}

Table S2. Fitted results of TRPL curves of the perovskite film deposited on FTO/SnO₂ substrate depending on 4-AMBA or 4-SABA treatment.

Sample	τ_1 (ns)	A_1 (%)	τ_2 (ns)	A_2 (%)	τ_{avg} (ns)
SnO ₂	153.12	11.77	515.74	88.23	501.93
SnO ₂ /4-AMBA	106.10	10.36	464.70	89.64	455.48
SnO ₂ /4-SABA	51.31	11.08	343.34	88.92	338.23

Table S3. Fitted results of UPS data and Tauc plot for estimating E_{VB} and E_{CB} .

Sample	$E_{cut-off}$ (eV)	E_F (eV)	$E_{F,edge}$ (eV)	E_{VB} (eV)	E_g (eV)	E_{CB} (eV)
SnO ₂	14.77	-6.45	3.34	-9.79	4.01	-5.78
SnO ₂ /4-AMBA	14.78	-6.44	3.23	-9.67	3.99	-5.68
SnO ₂ /4-SABA	14.81	-6.41	3.11	-9.52	3.99	-5.53
FAPbI ₃	16.08	-5.14	1.34	-6.48	1.52	-4.96

Table S4. Calculated EIS parameters of the devices with bare SnO₂, 4-AMBA modified SnO₂, and 4-SABA modified SnO₂.

Sample	R_s (Ωcm^2)	R_{ct} (Ωcm^2)	CPE (F)
SnO ₂	16.02	88.11	1.42×10^{-7}
SnO ₂ /4-AMBA	12.61	49.63	1.82×10^{-7}
SnO ₂ /4-SABA	5.92	36.84	6.70×10^{-8}