

Supporting Information for

Enhanced performance of perovskite solar cells via bilateral electron-donating passivator as a molecule bridge

Weichun Pan,^{§ a} Pengxu Chen,^{§ a} Sijia Zhu,^a Ruwei He,^a Qingshui Zheng,^a Fengxian Cao,^a

Zhang Lan,^a Jihuai Wu,^{* a} Weihai Sun,^{* a} and Yunlong Li^{* b}

^a *Engineering Research Center of Environment-Friendly Functional Materials, Ministry of Education, Institute of Materials Physical Chemistry, College of Materials Science & Engineering, Huaqiao University, Xiamen, 361021, China.*

^b *Shenzhen Institute of Advanced Technology Chinese Academy of Sciences, Shenzhen, China.*

This appendix include:

Figures S1~S15

Tables S1~S3

* Corresponding author: E-mail: jhwu@hqu.edu.cn; sunweihai@hqu.edu.cn; yl.li2@siat.ac.cn

§ These authors contributed equally to this work.

Figures S1-S15

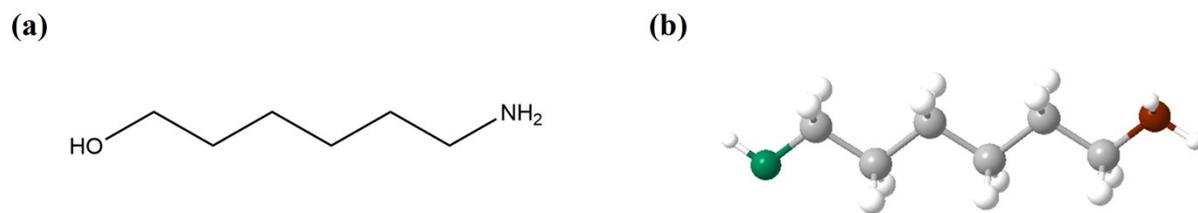


Figure S1. (a) The chemical structure of HAL. (b) The optimizing of geometries of HAL. The grey, white, green, and reddish brown atoms respectively represent the C, H, O, and N atoms.

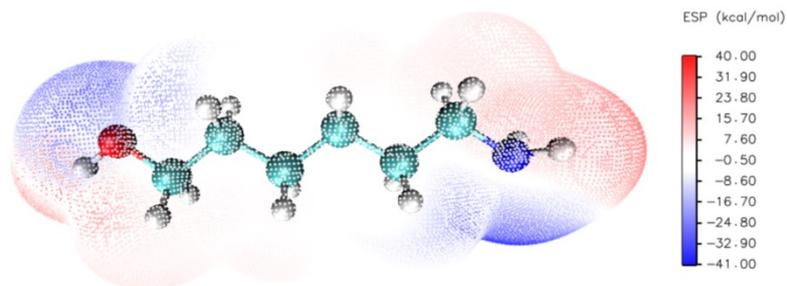


Figure S2. Electrostatic potential (ESP) map of HAL molecules.

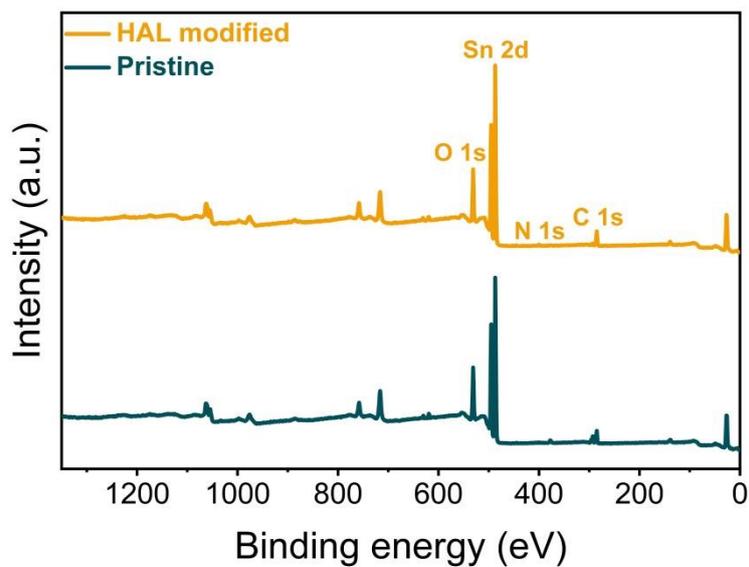


Figure S3. The XPS full spectra of the SnO₂ films without or with HAL modification.

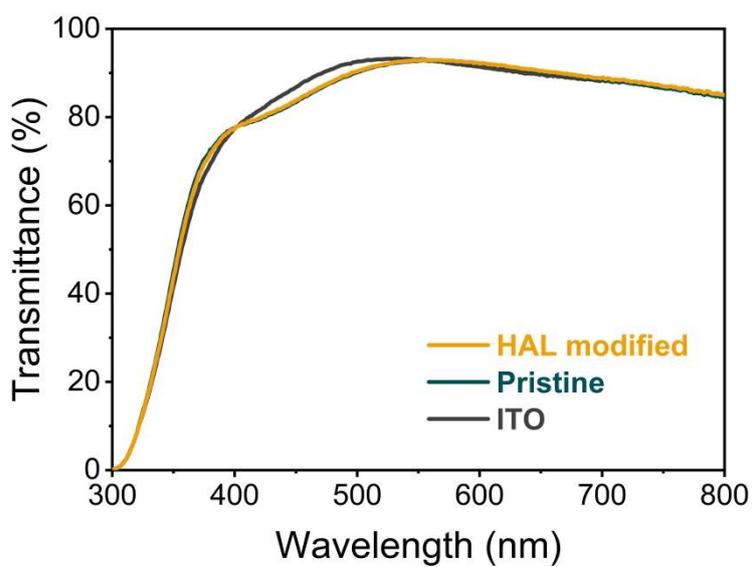


Figure S4. Transmittance spectra of the pristine SnO₂ film, HAL-modified SnO₂ film, and ITO substrate.

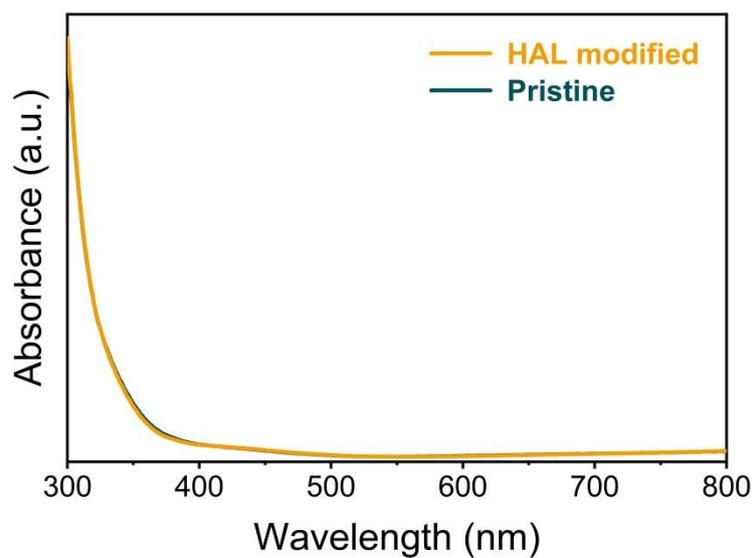


Figure S5. UV-vis absorption spectra of the SnO₂ films without or with HAL modification.

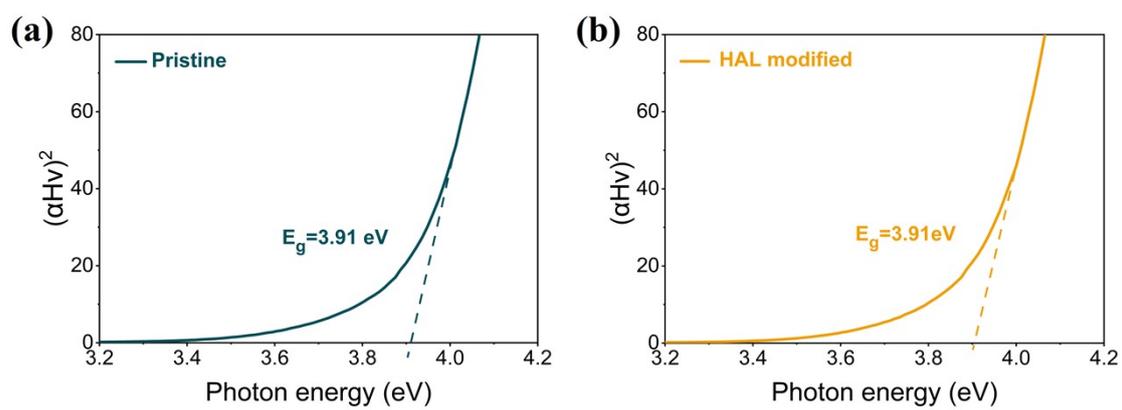


Figure S6. Optical band gap energy (E_g) of the (a) pristine SnO₂ and (b) HAL-modified SnO₂ films.

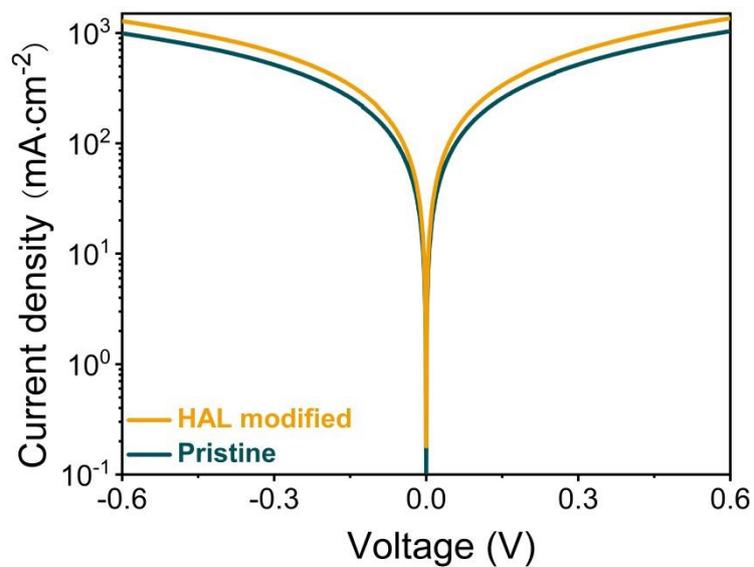


Figure S7. The Tafel curves of devices with a structure of ITO/SnO₂ (without and with HAL)/Au.

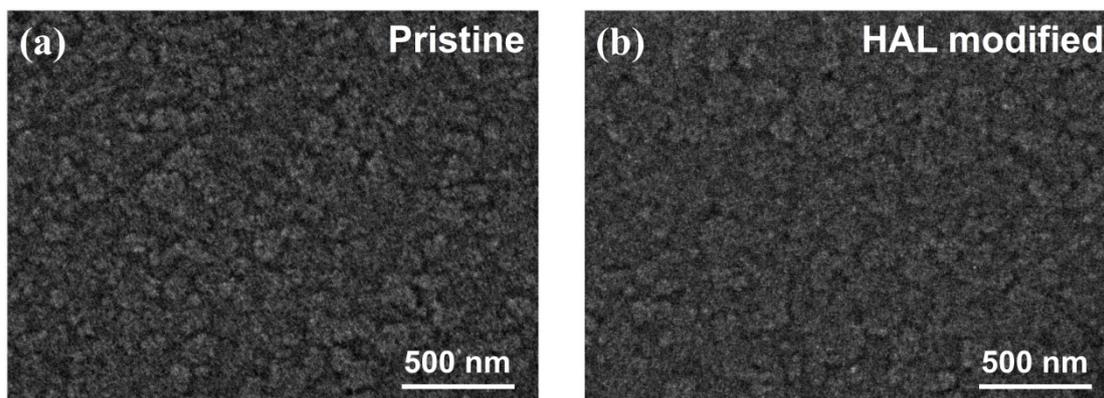


Figure S8. Top-view SEM images of the (a) pristine SnO₂ and (b) HAL-modified SnO₂ films.

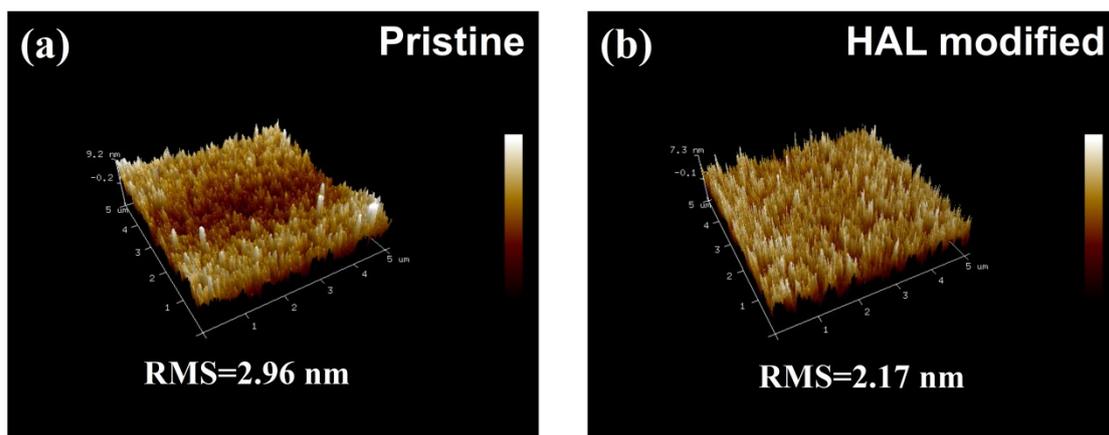


Figure S9. The AFM images of the (a) pristine SnO₂ and (b) HAL-modified SnO₂ films.

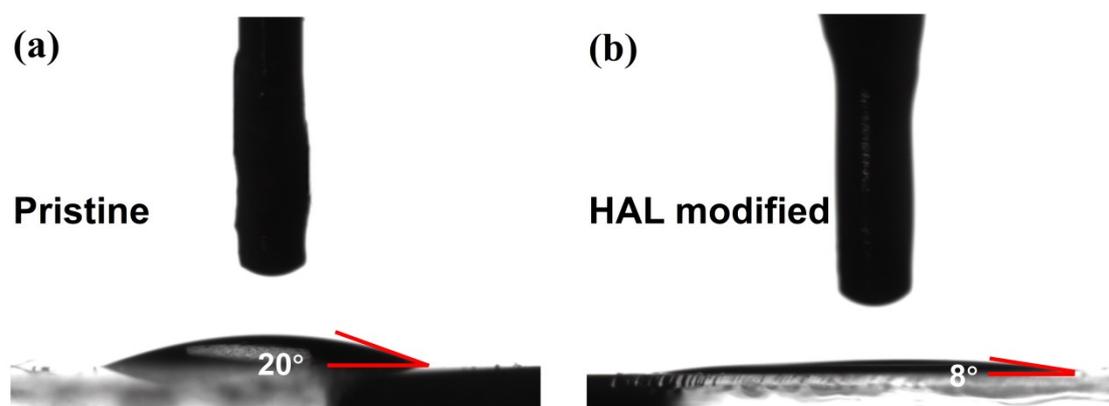


Figure S10. The contact angle measurements of the DMF/DMSO mixture solution on the (a) pristine SnO₂ and (b) HAL-modified SnO₂ substrates.

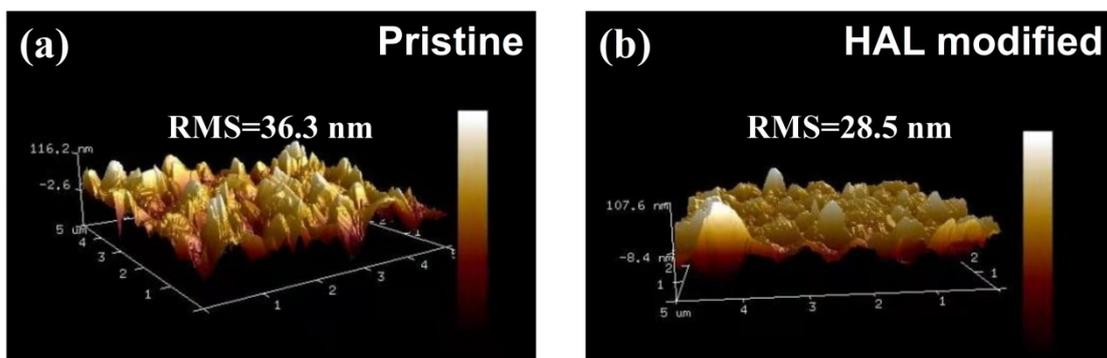


Figure S11. The AFM images of perovskite films on the (a) pristine SnO₂ and (b) HAL-modified SnO₂ films.

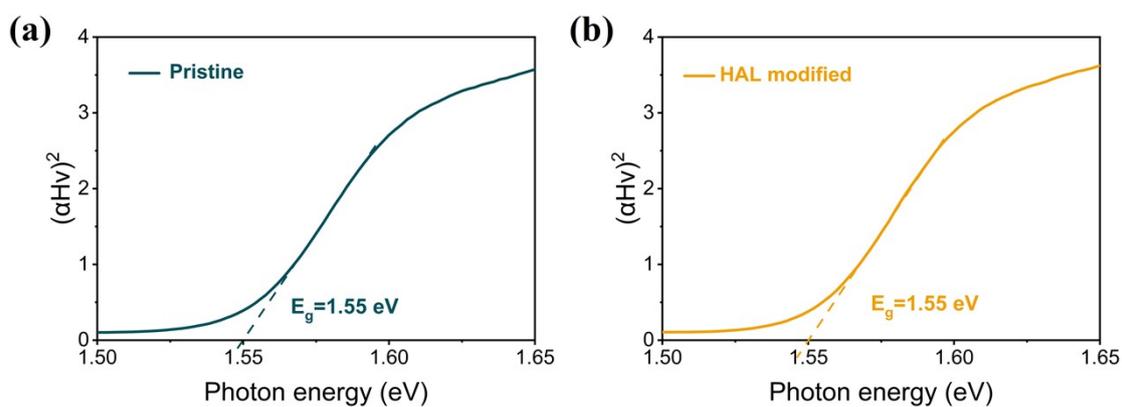


Figure S12. Optical band gap energy (E_g) of perovskite films on the (a) pristine SnO₂ and (b) HAL-modified SnO₂ films.

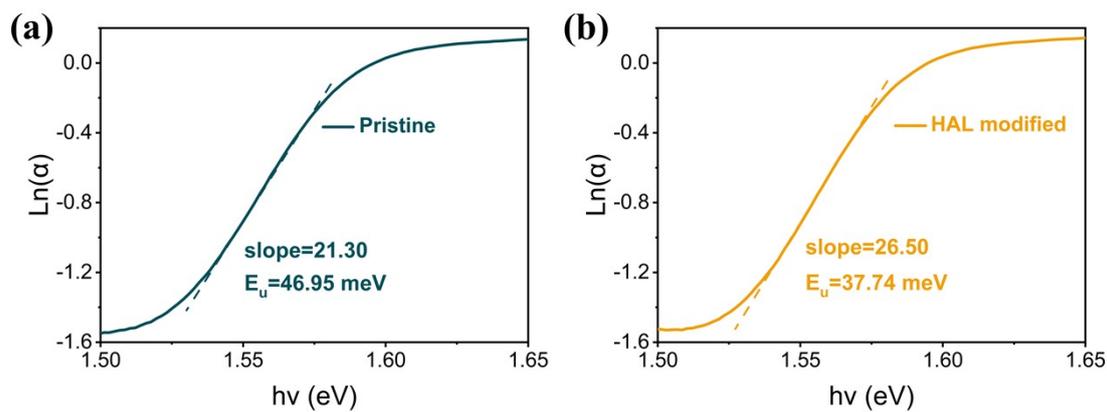


Figure S13. Logarithm of absorption coefficient (α) versus photon energy and the Urbach energy calculated in the perovskite based on the (a) pristine SnO_2 and (b) HAL-modified SnO_2 films.

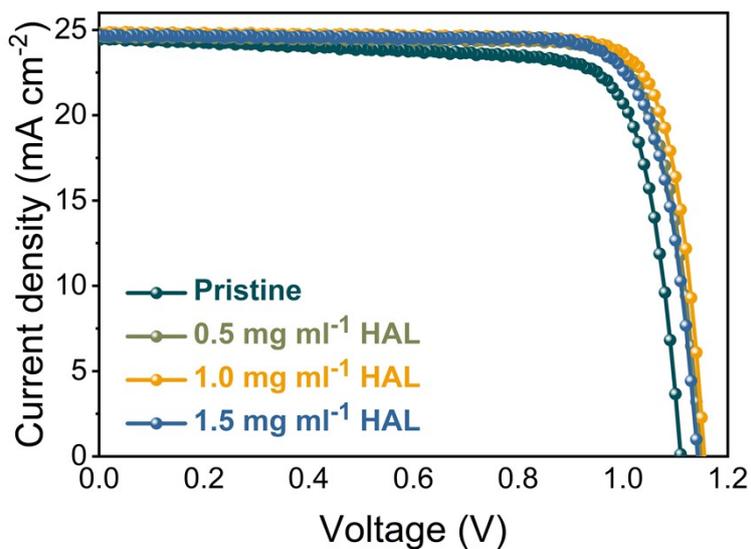


Figure S14. J - V curves of the pristine device and the devices modified with different concentrations of HAL solutions.

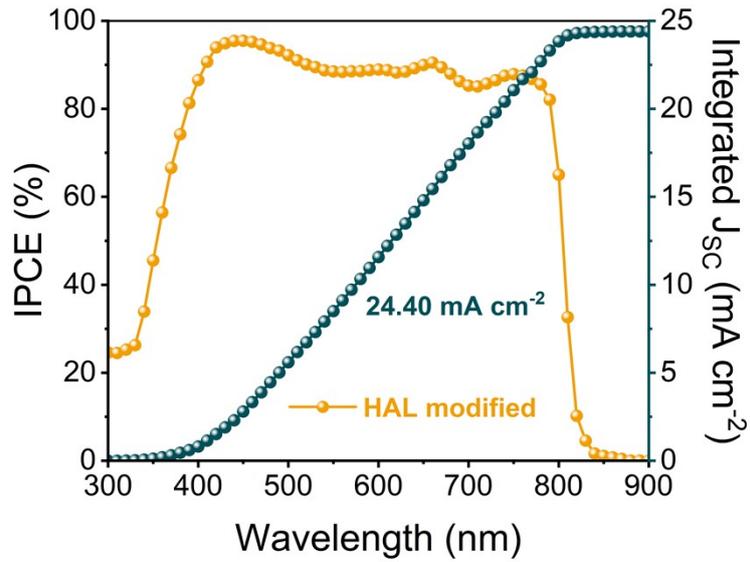


Figure S15. EQE spectrum and integrated current density of the HAL-modified device. The integrated current density is 24.40 mA cm^{-2} .

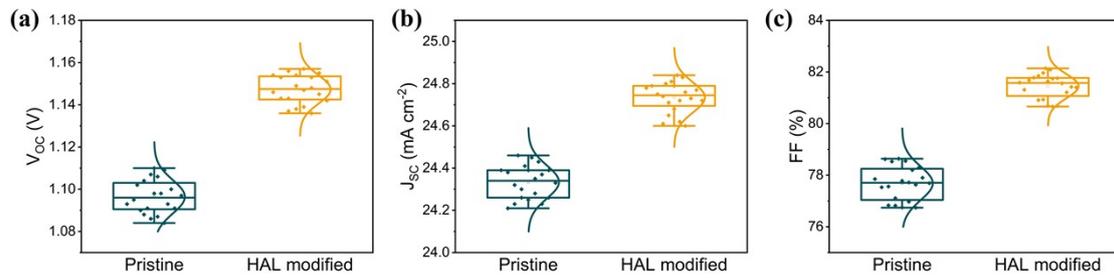


Figure S16. (a) V_{OC} , (b) J_{SC} , and (c) FF statistical diagrams of pristine and HAL-modified devices.

Tables S1-S3

Table S1 Energy levels of pristine SnO₂ film and HAL-modified SnO₂ film.

Samples	E _{cutoff} (eV)	W _F (eV)	E _{onset} (eV)	E _{VBM} (eV)	E _{CBM} (eV)	E _g (eV)
Pristine	16.76	4.46	3.73	-8.19	-4.28	3.91
HAL-modified	16.68	4.54	3.76	-8.30	-4.39	3.91

Table S2 TRPL parameters of perovskite on SnO₂ films without or with HAL modification from Figure 3d.

Samples	τ_{avg} (ns)	τ_1 (ns)	τ_2 (ns)	A ₁ (%)	A ₂ (%)
Pristine	96.56	35.93	113.41	21.74	78.26
HAL-modified	64.36	22.39	78.58	25.30	74.70

Table S3. Electrical impedance of the PSCs without or with HAL modification.

Samples	R _s (Ω)	R _{ct} (Ω)	R _{rec} (Ω)
Pristine	11.55	54.09	28.32
HAL-modified	10.84	24.45	90.07

Table S4 Photovoltaic data of PSCs based on SnO₂ films without or with HAL modification.

Samples	V _{OC} (V)	J _{SC} (mA cm ⁻²)	FF (%)	PCE (%)
Pristine	1.110	24.41	78.61	21.30
0.5 mg mL ⁻¹	1.148	24.66	81.19	22.99
1.0 mg mL ⁻¹	1.155	24.82	82.27	23.58
1.5 mg mL ⁻¹	1.142	24.75	80.90	22.87

Table S5 Photovoltaic data statistics of 20 PSCs based on SnO₂ films without or with HAL modification.

Samples	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE (%)
Pristine	1.095±0.008	24.33±0.08	77.69±0.65	20.73±0.25
HAL-modified	1.147±0.007	24.74±0.07	81.45±0.47	23.11±0.22