Supporting information

Molecule-bridged Electron-selective Contact for High-efficient Halide-based Perovskite Solar Cells†

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† Electronic supplementary information (ESI) available.

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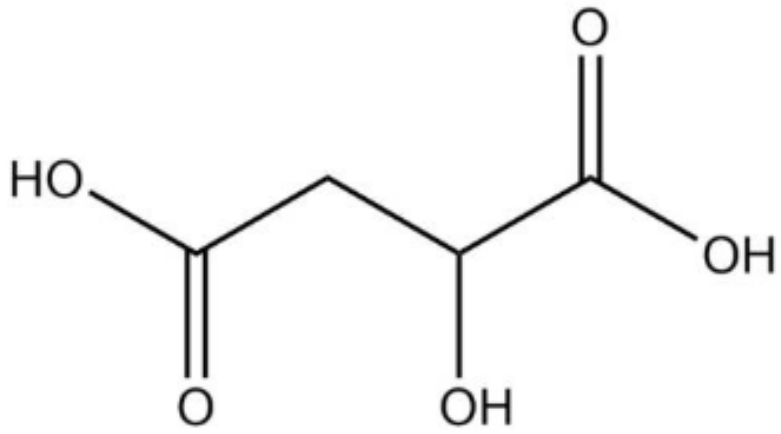

Fig. S1. Structure diagram of the molecular formula of H_2Mi.

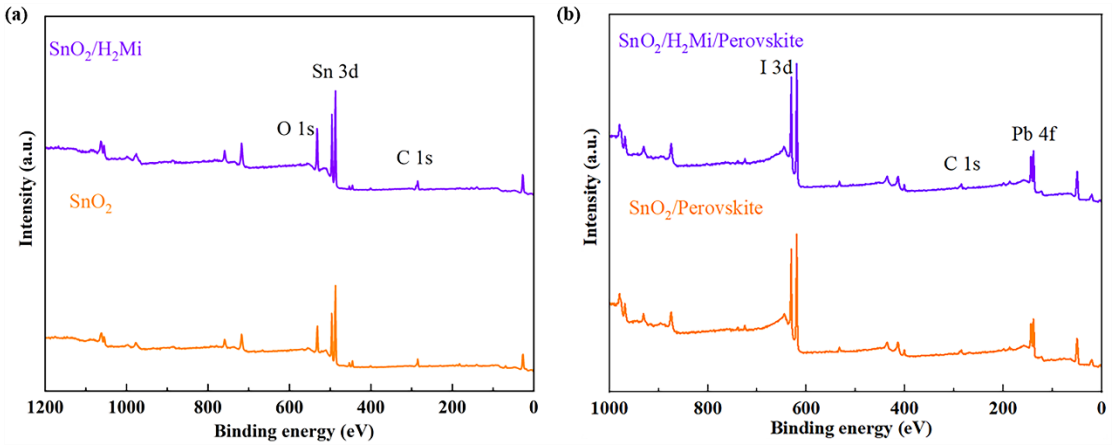

Fig. S2. (a) XPS full spectra of SnO_2 and SnO_2/H_2Mi. (b) XPS full spectra of SnO_2/Perovskite and SnO_2/H_2Mi/Perovskite.

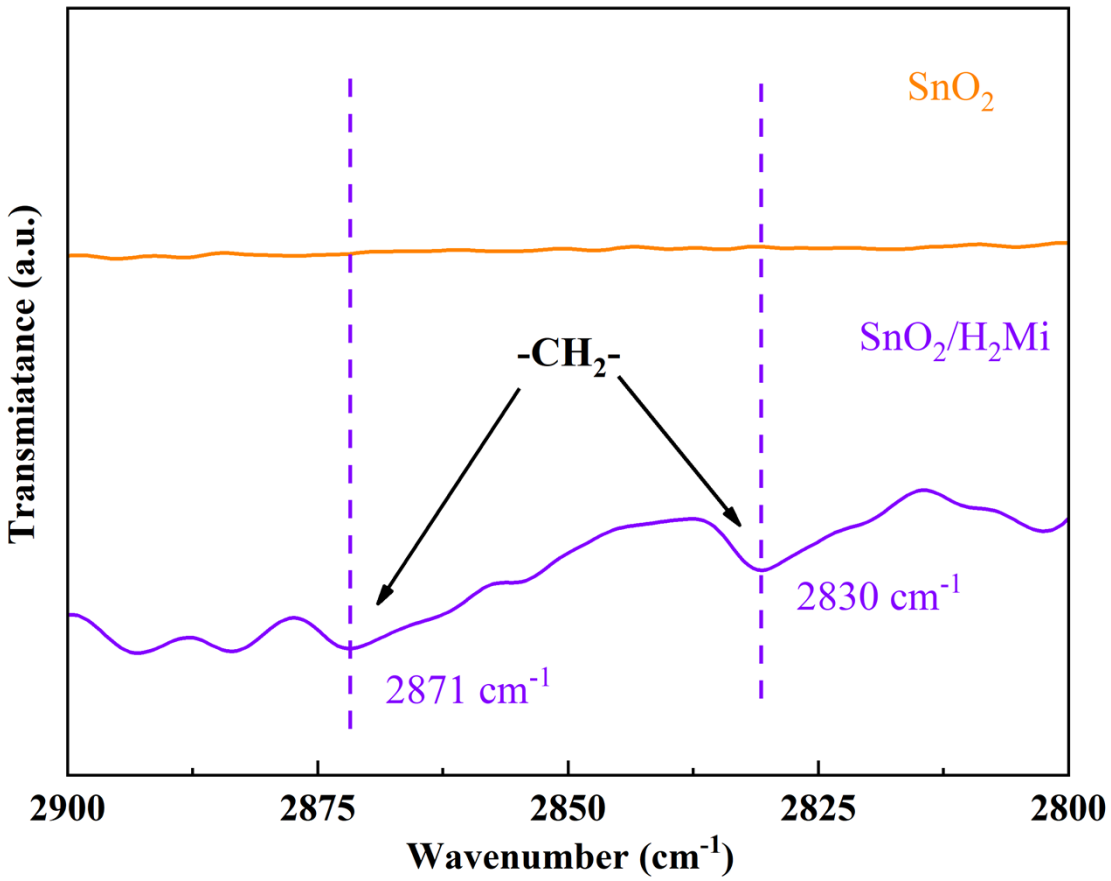

Fig. S3. FTIR spectra of SnO_2 and SnO_2/H_2Mi.

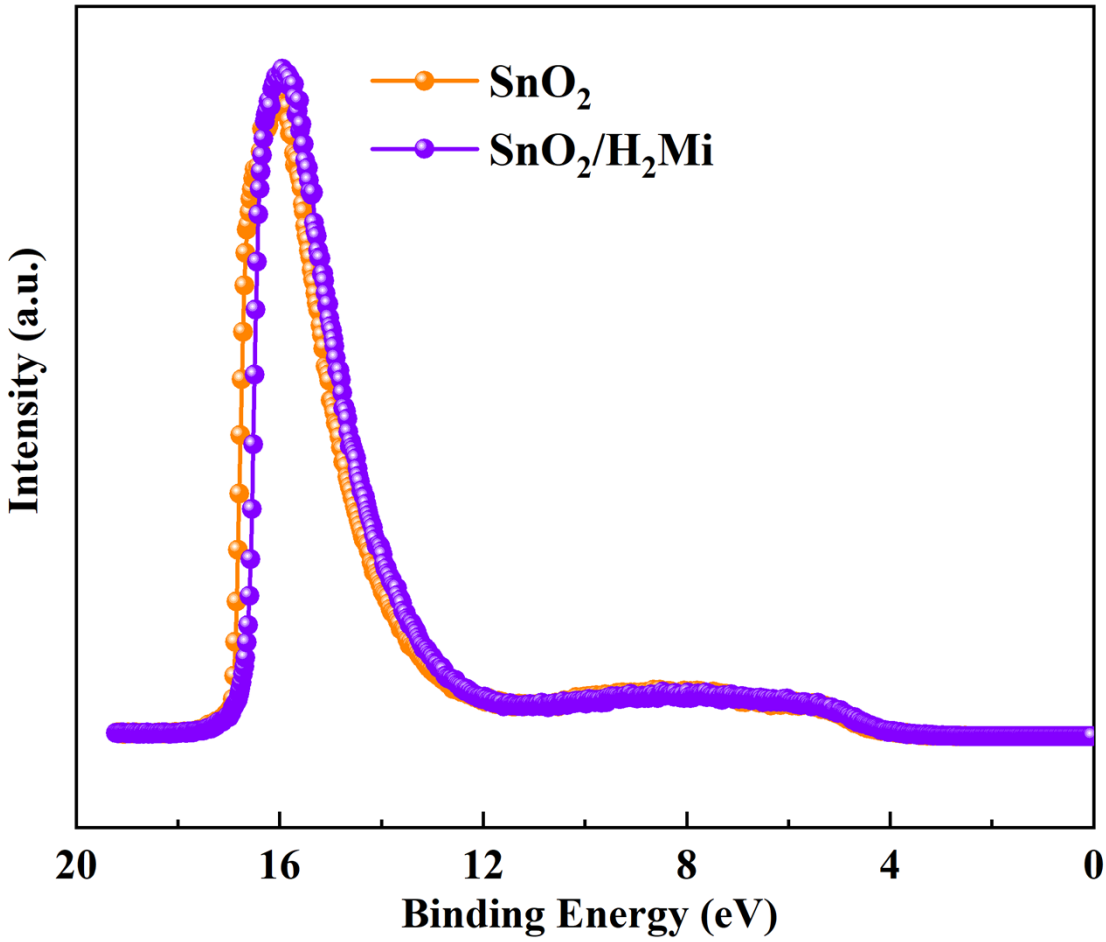

Fig. S4. UPS full spectra of SnO_2 and SnO_2/H_2Mi films.

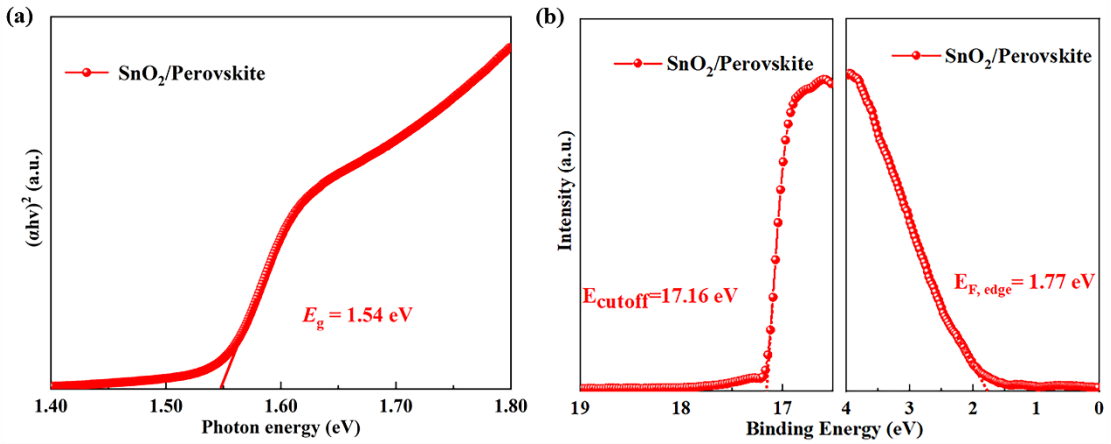

Fig. S5. (a) Tauc-Plot spectrum of perovskite films deposited on SnO_2/Perovskite substrate. (b) UPS spectra of SnO_2/Perovskite film.

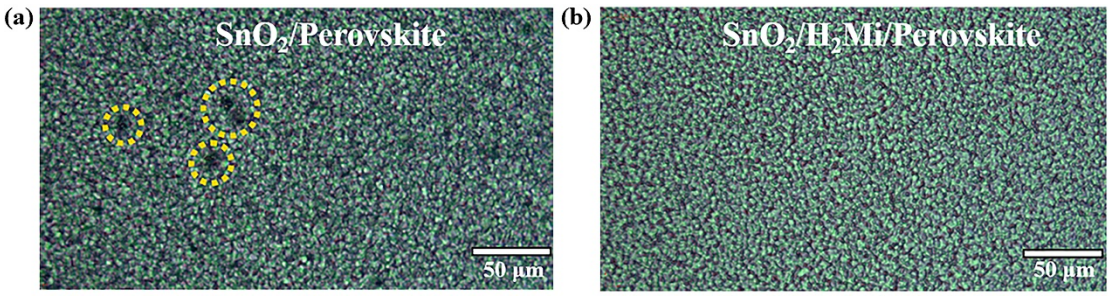

Fig. S6. OM images of perovskite films deposited on (a) SnO_2 and (b) SnO_2/ H_2Mi ETLs.

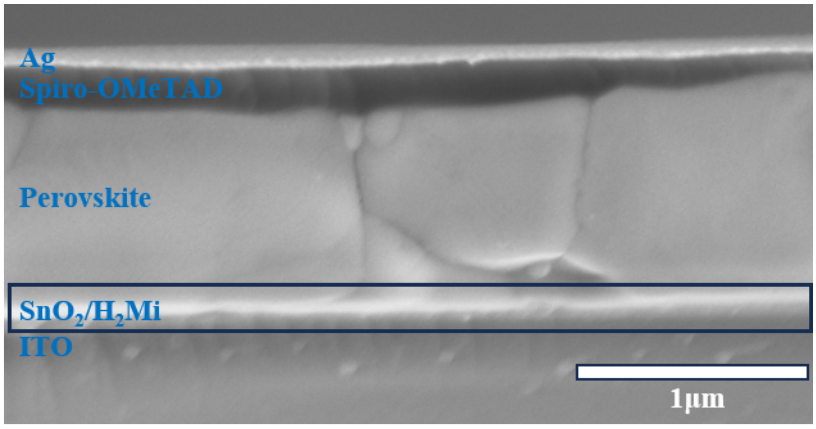

Fig. S7. The cross-sectional SEM images of the perovskite film treated with H_2Mi.

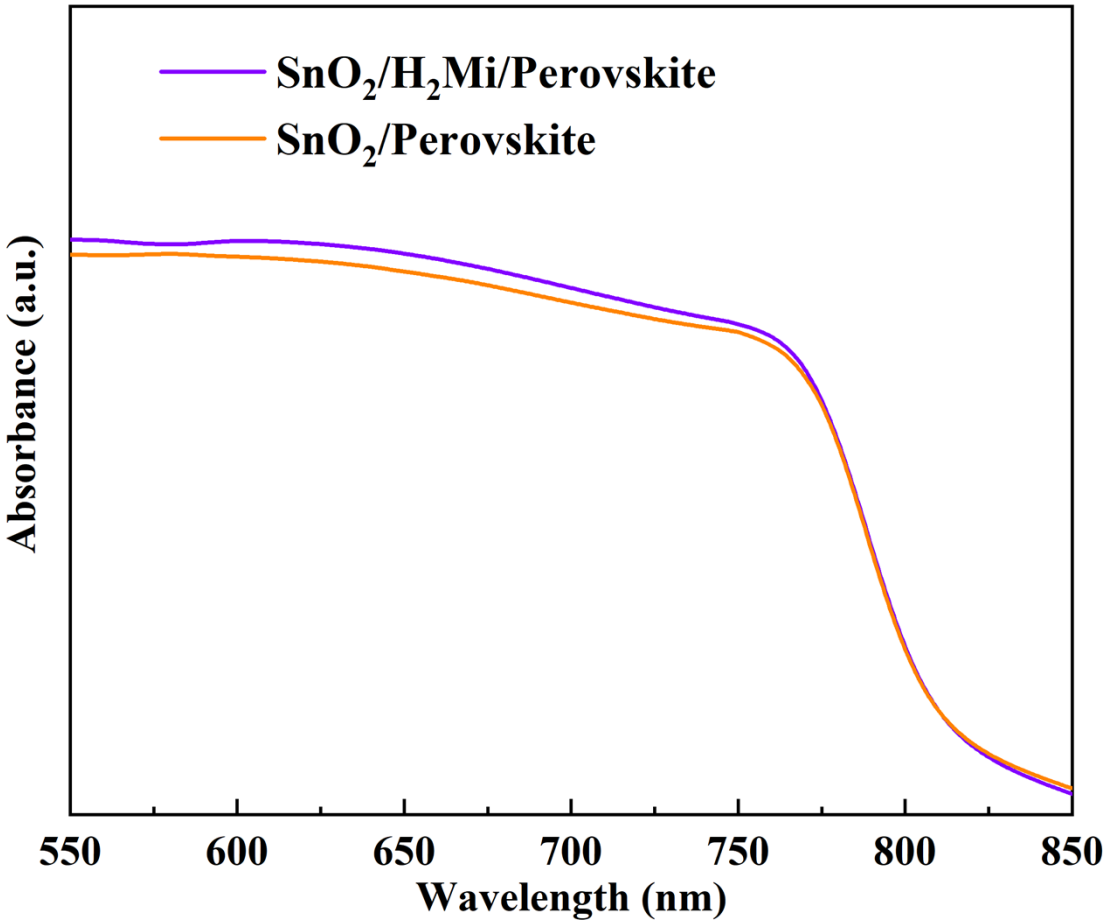

Fig. S8. UV/vis absorption spectra of perovskite films deposited on SnO_2 and SnO_2/H_2Mi ETLs.

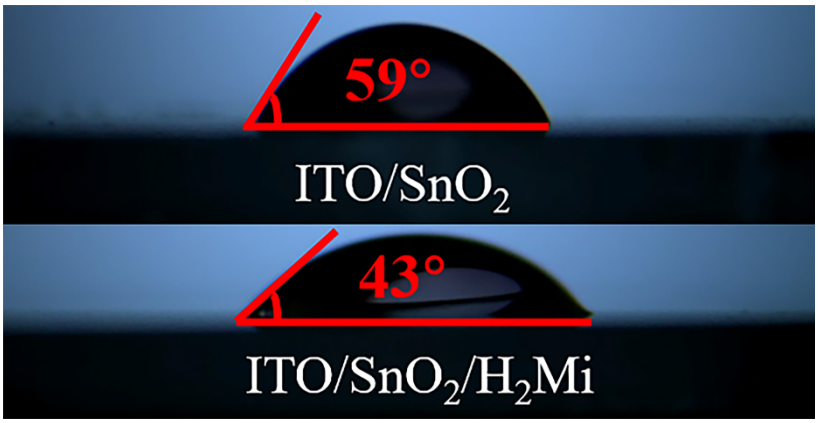

Fig. S9. The contact angle measurements of ITO/SnO_2 and ITO/SnO_2 /H_2Mi films.

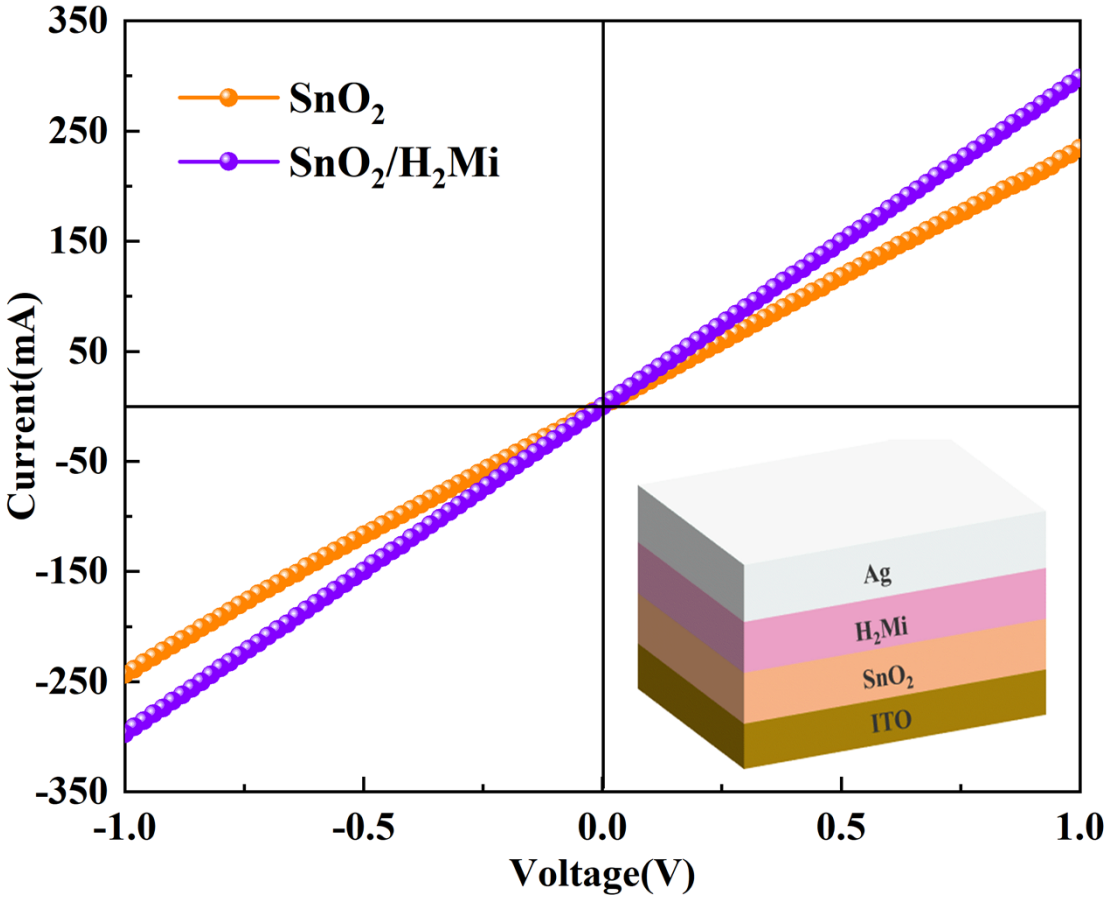

Fig. S10. I−V curves of devices based on SnO_2 and SnO_2/H_2Mi ETLs. The inset depicts the device structure.

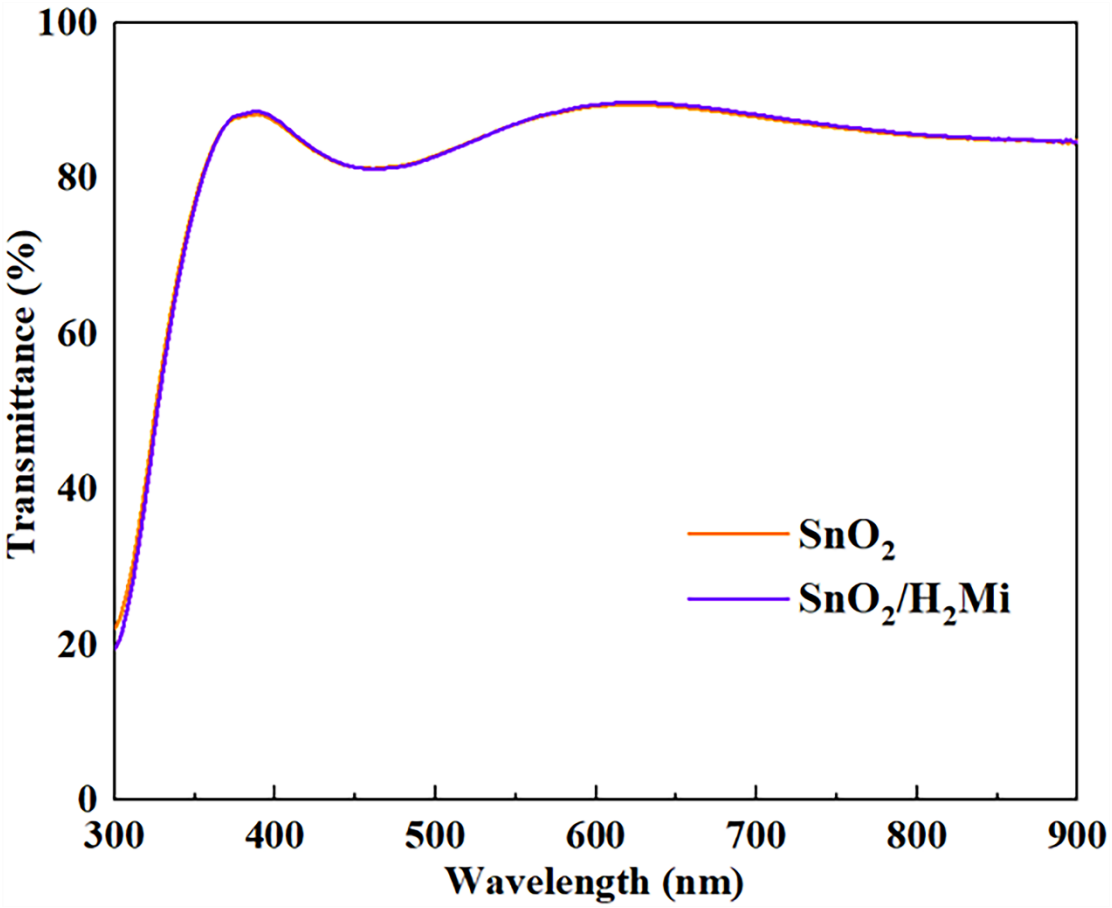

Fig. S11. UV-vis absorption spectra of SnO2 and SnO2/ H2Mi ETLs.

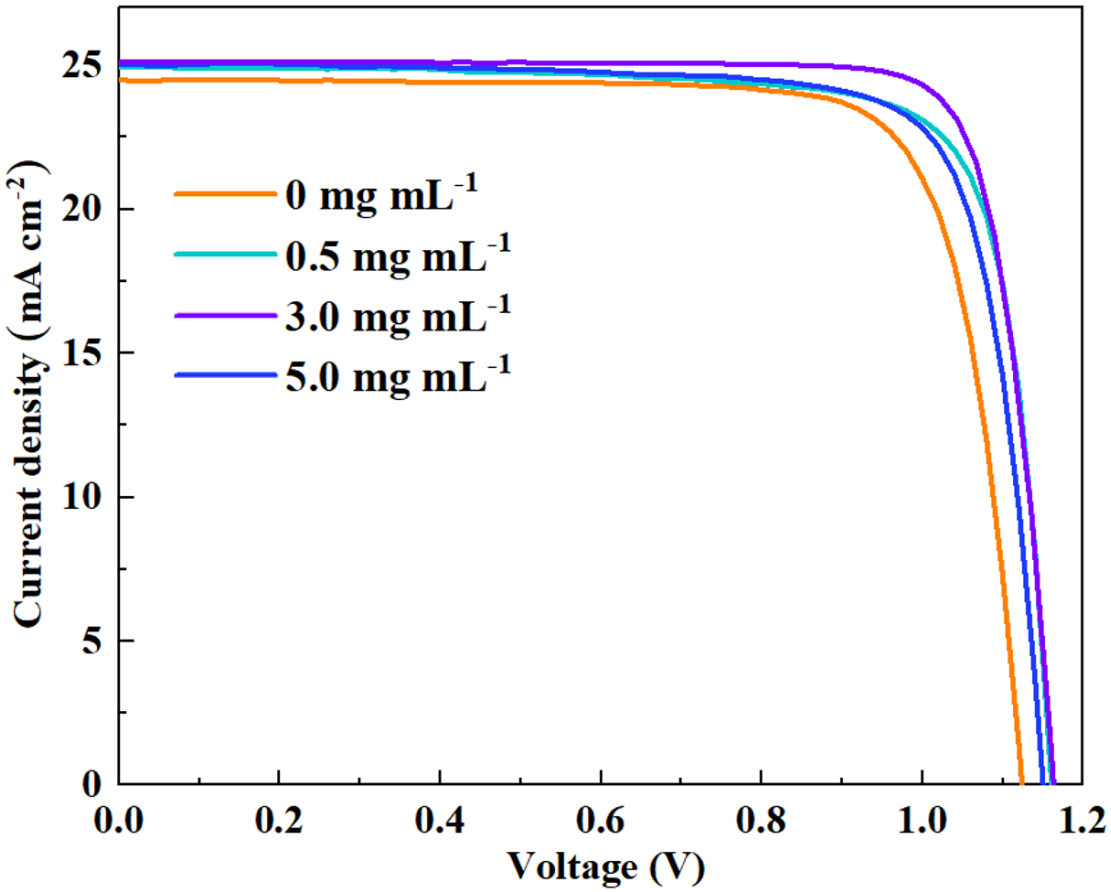

Fig. S12. J-V curves of the device based on SnO_2 passivated with different concentrations of H_2Mi.

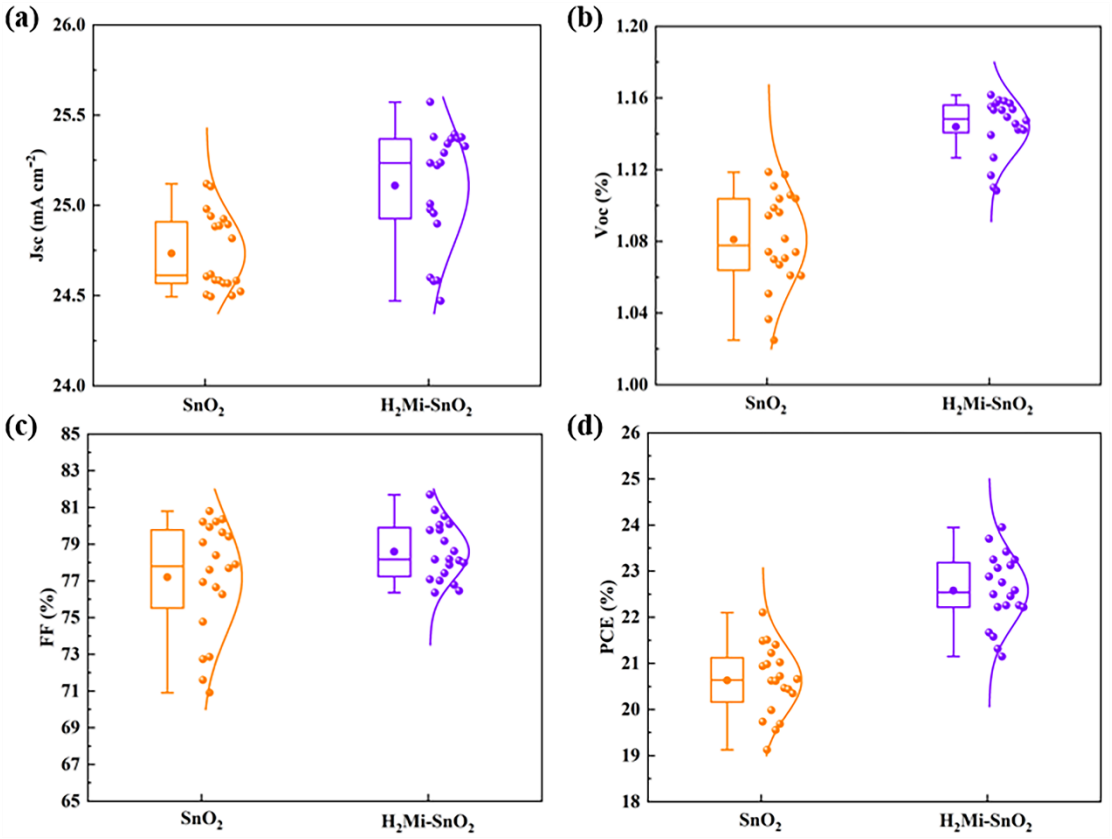

Fig. S13. The box plots of (a) J_{SC}, (b) V_{OC}, (c) FF, and (d) PCE of the unencapsulated devices.

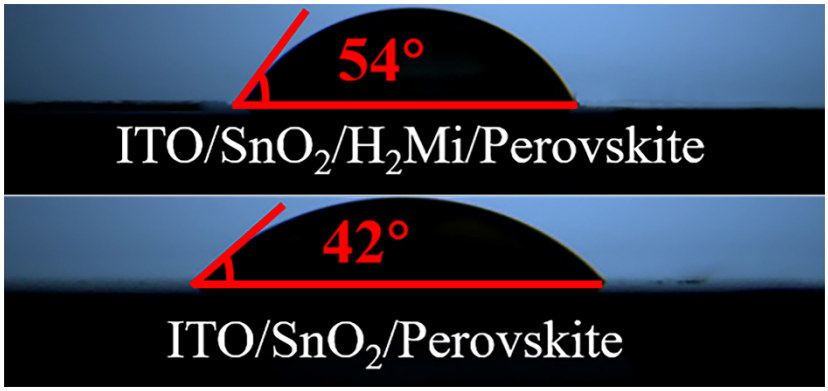

Fig. S14. The contact angle measurements of perovskite precursor solution on ITO/SnO_2 and $ITO/SnO_2/H_2Mi$.

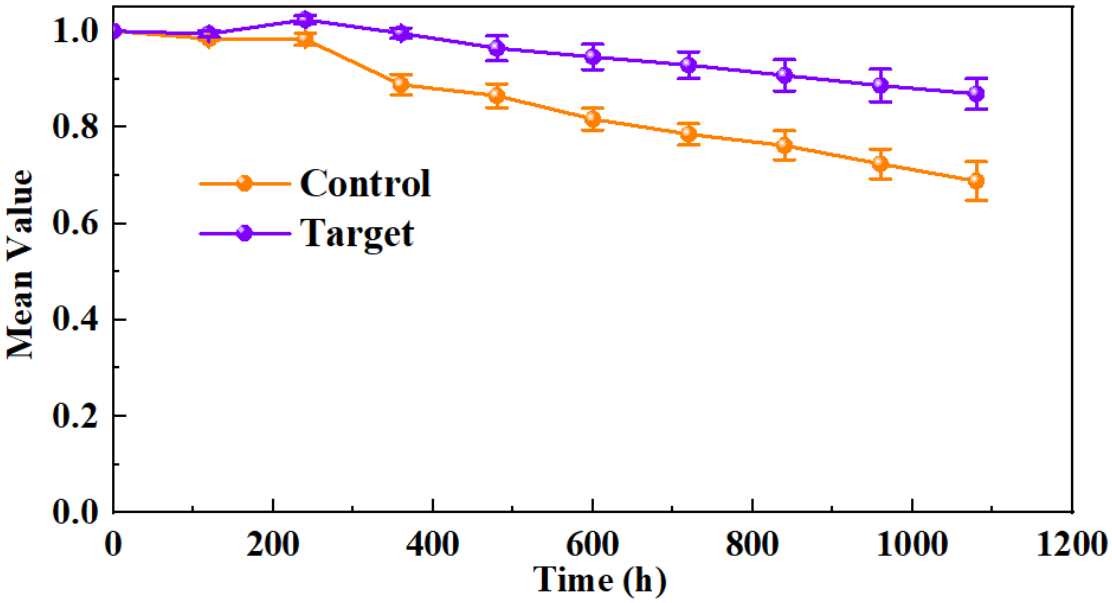

Fig. S15. The environmental stability curves of the control and H2Mi-modified devices

Table S1. Calculated parameters for the energy level of SnO_2, SnO_2/H_2Mi, and perovskite.

Sample	E_{cutoff} (eV)	W_F (eV)	$E_{F, edge}$ (eV)	E_{VB} (eV)	E_g (eV)	E_{CB} (eV)
SnO_2	**16.61**	**4.61**	**3.92**	**-8.53**	**3.90**	**-4.63**
SnO_2/H_2Mi	**16.88**	**4.34**	**4.06**	**-8.40**	**3.91**	**-4.49**
Perovskite	**17.16**	**4.06**	**1.77**	**-5.83**	**1.54**	**-4.29**

Table S2. Calculated average crystallite sizes of perovskite with and without H_2Mi modification according to Scherrer formula.

	2Theta(°)	FWHM(°)	D (nm)
Control-Perovskite	**14.22**	**0.144**	**54.98**
Target-Perovskite	**14.22**	**0.119**	**66.53**

Table S3. The fitted data of TRPL curves.

Sample	τ_1 (ns)	τ_2 (ns)	A_1	A_2	τ_{ave}(ns)
SnO_2/Perovskite	**119.71**	**813.74**	**168.3**	**1590.79**	**803.11**
SnO_2/Perovskite /H_2Mi	**100**	**795.64**	**89.23**	**832.59**	**786.4**

Table S4. Performance summary of champion devices based on SnO_2 and SnO_2 passivated with different concentrations of H_2Mi.

	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
0 mg mL^{-1}	**1.12**	**24.48**	**79.00**	**21.71**
0.5 mg mL^{-1}	**1.16**	**24.96**	**79.77**	**23.07**
3.0 mg mL^{-1}	**1.16**	**25.12**	**83.35**	**24.34**
5.0 mg mL^{-1}	**1.15**	**25.01**	**79.17**	**22.76**

Table S5. The photovoltaic parameters of the PSCs prepared with and without H_2Mi modification were measured in the reverse scan (RS) and forward scan (FS)

	Sweep direction	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)	Hysteresis index
Control	Reverse	1.12	24.48	79.00	21.71	0.072
	Forward	1.06	24.59	77.41	20.15	
Target	Reverse	1.16	25.12	83.35	24.34	0.038
	Forward	1.16	25.29	80.04	23.42	

Table S6. The initial photovoltaic parameters of three groups of PSCs devices before and after H2Mi modification were tested for environmental stability.

Groups	Sample	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
Groups 1	Control	1.05	24.62	79.94	20.63
	Target	1.15	25.34	80.09	23.25
Groups 2	Control	1.08	24.63	78.54	20.87
	Target	1.16	25.29	80.05	23.42
Groups 3	Control	1.11	24.78	74.51	20.58
	Target	1.15	24.90	80.52	23.13