

## Supplementary Information

### **Surface pre-sacrifice behavior of thiourea-based 2D perovskite for high-performance perovskite solar cells**

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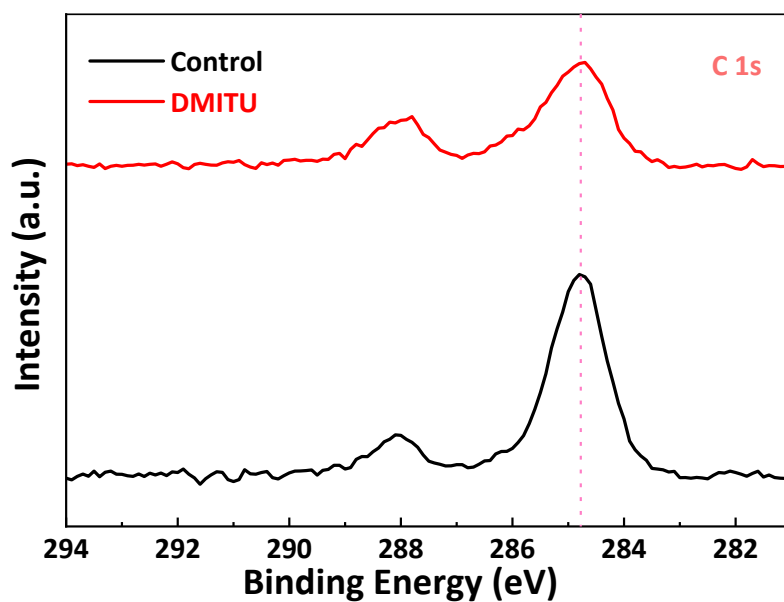


Fig. S1 XPS spectra of C 1s for the control and DMITU perovskite films.

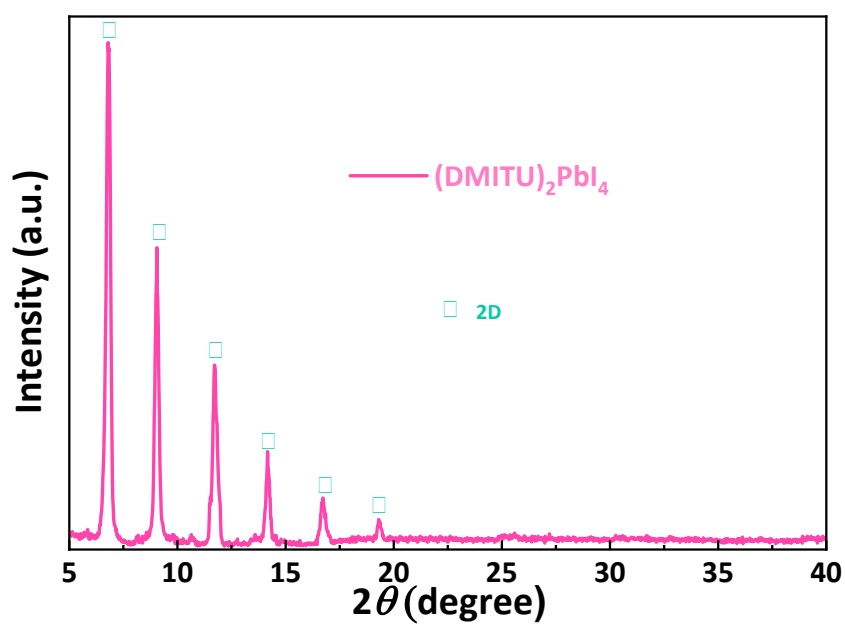
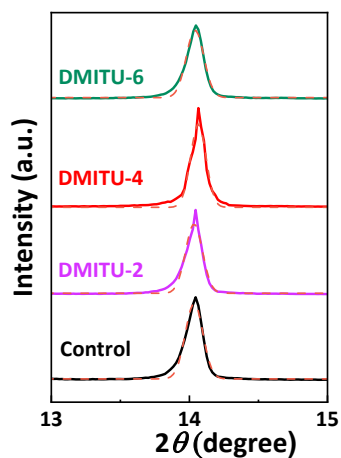
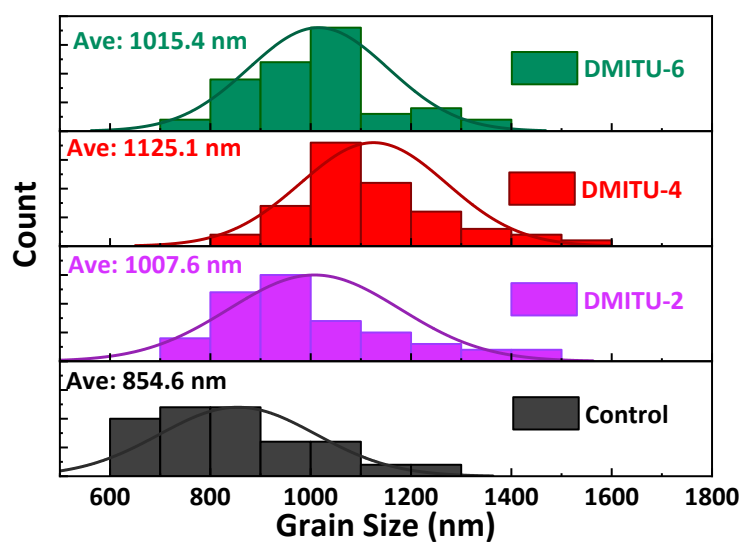


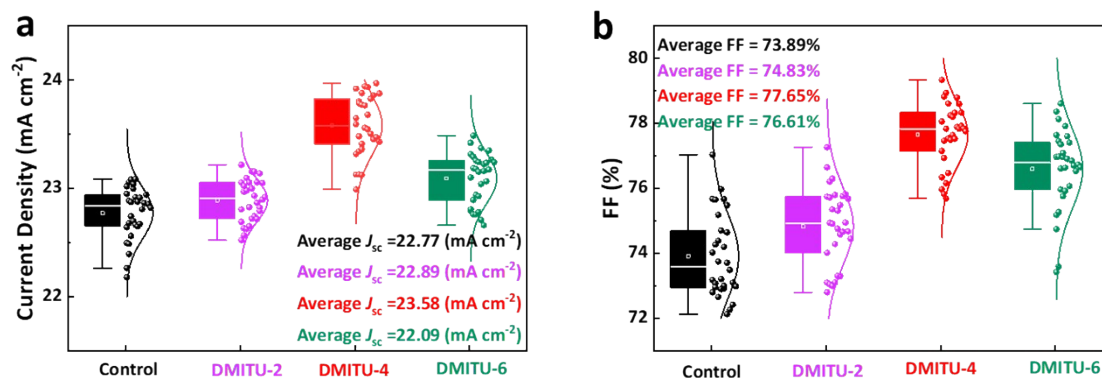
Fig. S2 XRD pattern of (DMITU)<sub>2</sub>PbI<sub>4</sub> (n=1) perovskite film.



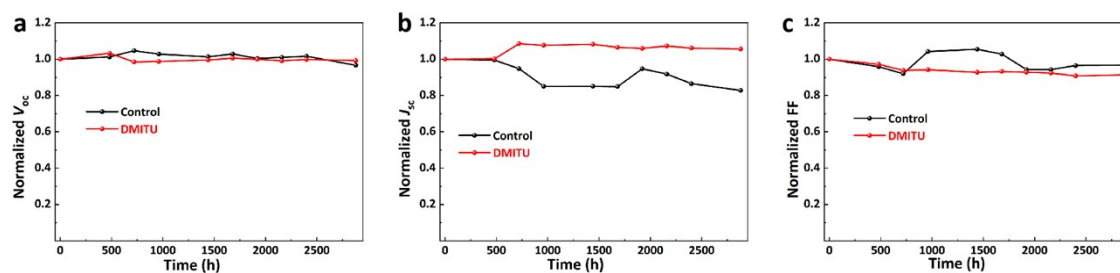
**Fig. S3** The magnified XRD patterns with Gaussian fit for the control and DMITU PSCs with different concentrations.



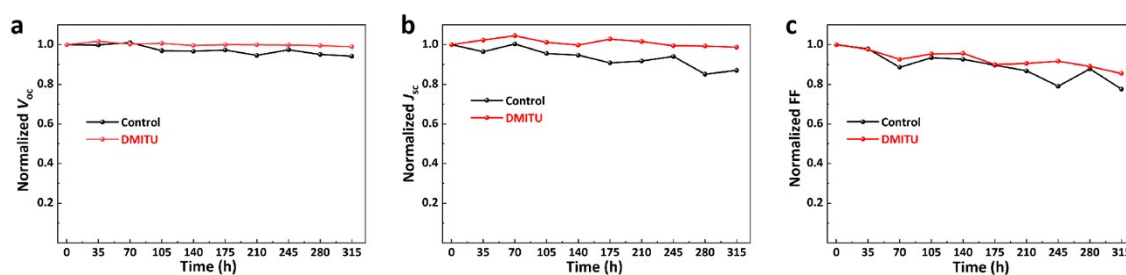
**Fig. S4** The statistic distributions of the grain sizes for the control, DMITU-2, DMITU-4 and DMITU-6 perovskite films.



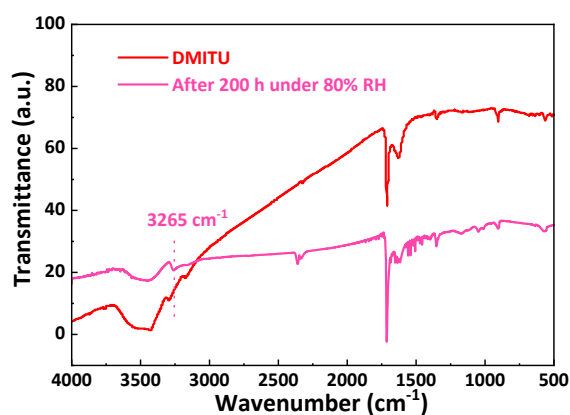
**Fig. S5** (a)  $J_{sc}$  and (b) FF distributions of the control, DMITU-2, DMITU-4 and DMITU-6 perovskite devices.



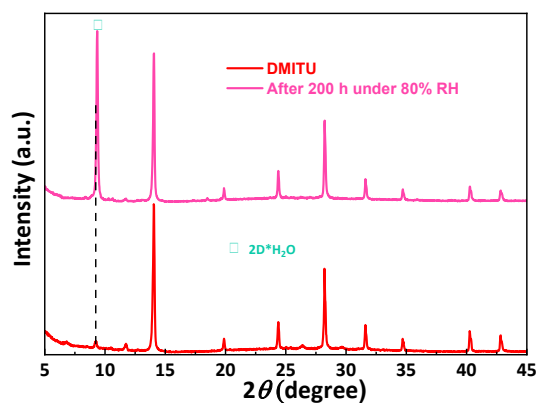
**Fig. S6** Normalized (a)  $V_{oc}$ , (b)  $J_{sc}$  and (c) FF variation curves of the unsealed control and DMITU PSCs aging under 50% RH for 2880 h.



**Fig. S7** Normalized (a)  $V_{oc}$ , (b)  $J_{sc}$  and (c) FF variation curves of the unsealed control and DMITU PSCs aging at 85 °C for 315 h.



**Fig. S8** FTIR spectra of the perovskite + DMITU film before and after aging under 80% RH for 200 h.



**Fig. S9** XRD patterns for the DMITU perovskite film before and after aging under about 80% RH for 200 h.

**Table S1** Photovoltaic parameters of the control and DMITU PSCs with different concentrations.

Device	$V_{oc}$ (V)	$J_{sc}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
Control	1.14	23.02	77.05	20.18
DMITU-2	1.17	23.06	77.23	20.78
DMITU-4	1.17	23.92	79.34	22.26
DMITU-6	1.17	23.42	78.37	21.51
DMITU-8	1.14	23.00	73.47	19.21

**Table S2** Photovoltaic parameters of the control and DMITU PSCs under reverse and forward scan directions.

Device	$V_{oc}$ (V)	$J_{sc}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
Control-Reverse	1.14	23.02	77.05	20.18
Control-Forward	1.12	23.05	73.27	18.95
DMITU-Reverse	1.17	23.92	79.34	22.26
DMITU-Forward	1.17	23.68	78.90	21.86

**Table S3** The intensities and FWHM values of the (110) crystal plane for the control and DMITU PSCs with different concentrations.

Device	Intensity (a.u.)	FWHM
Control	19236	0.12733
DMITU-2	20013	0.12304
DMITU-4	22947	0.11202
DMITU-6	17037	0.12788