

## Supporting Information

# Effective n-Type De-doping of Perovskite Surface by Defect Passivation and Improved Film Crystallization for High-Efficiency Inorganic Solar Cells

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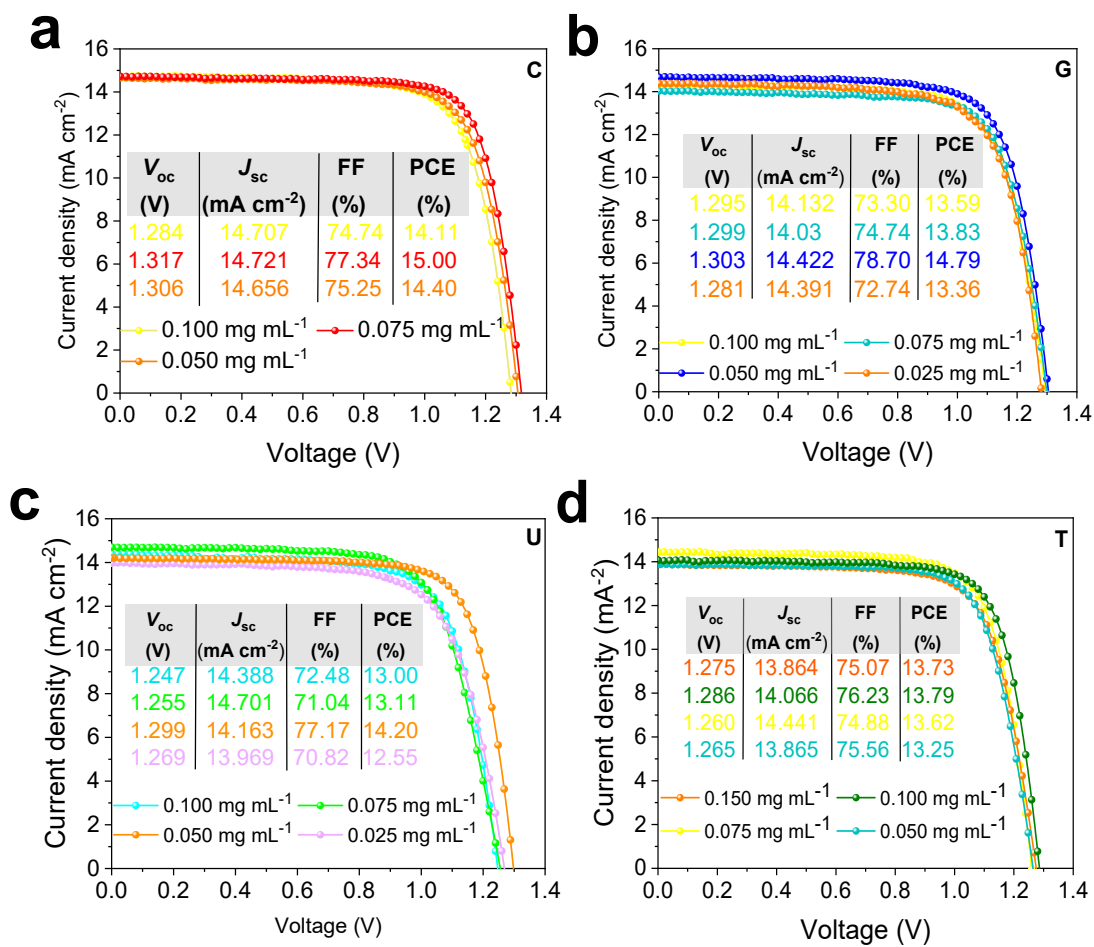
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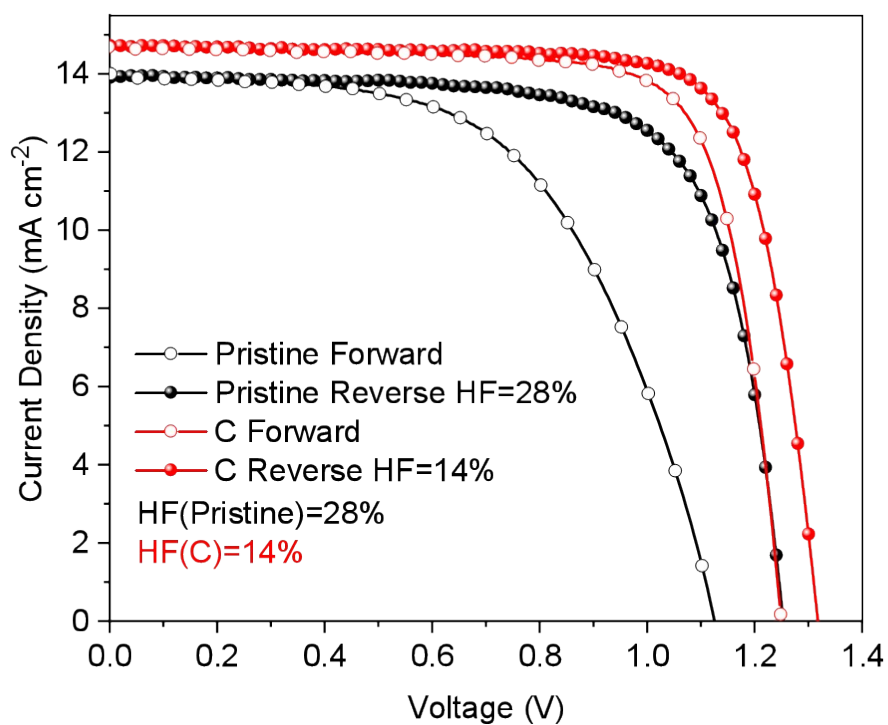
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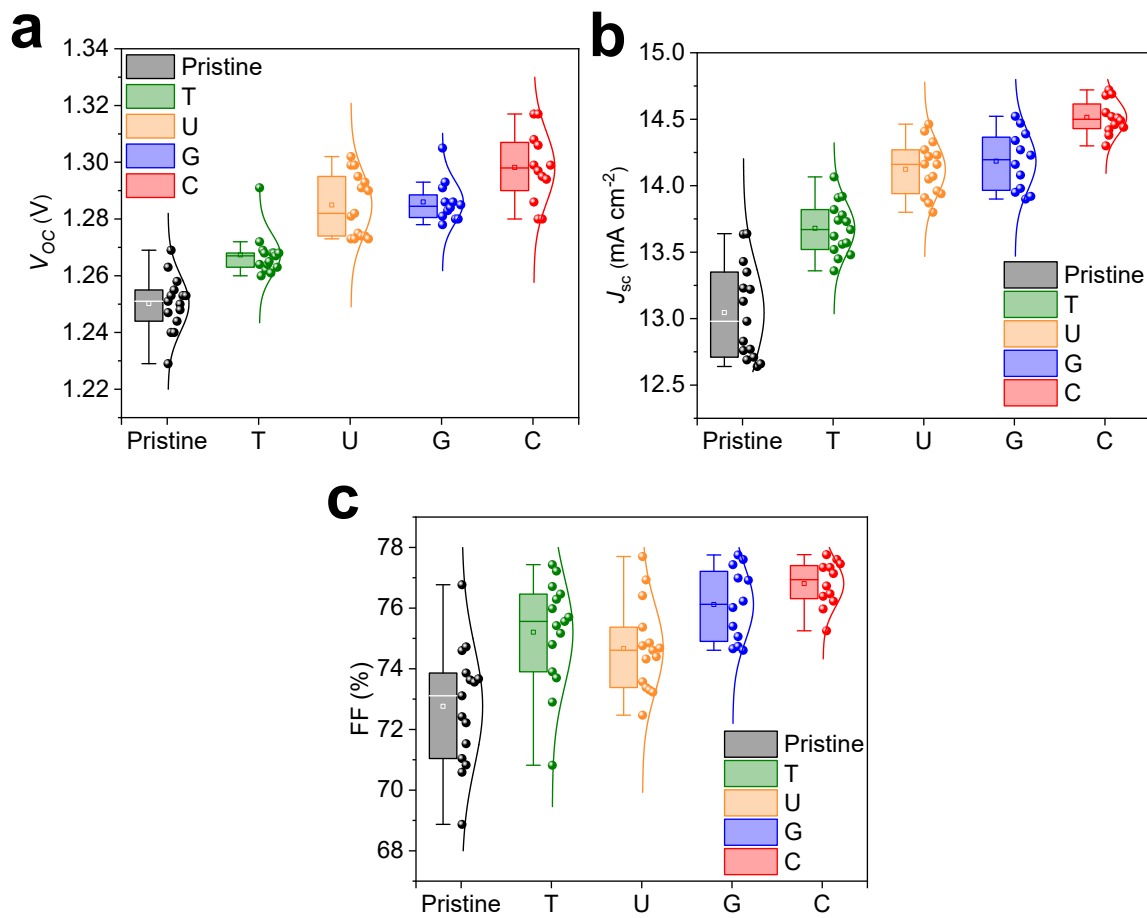
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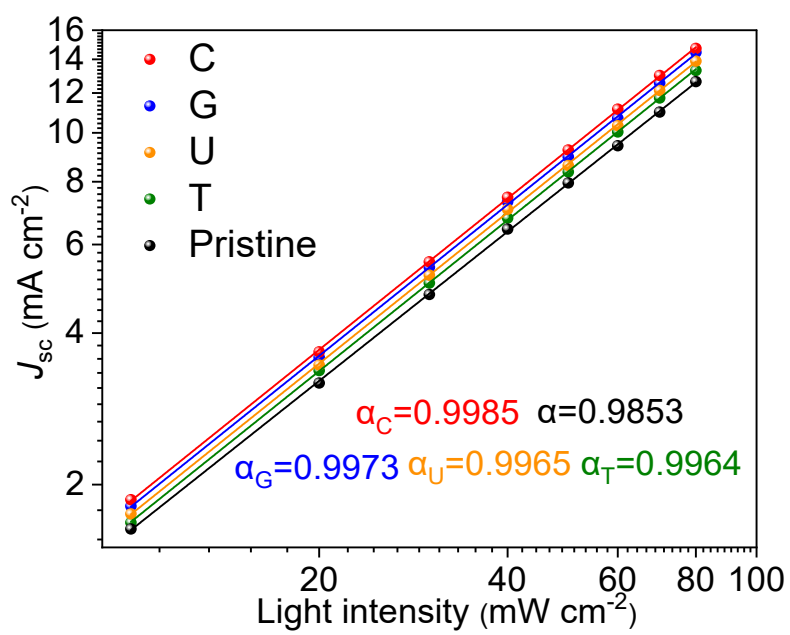
**Fig. S1**  $J$ - $V$  curves of the prepared  $\text{CsPbI}_2\text{Br}$  devices treated by (a) cytosine (b) guanine (c) uracil (d) thymine.



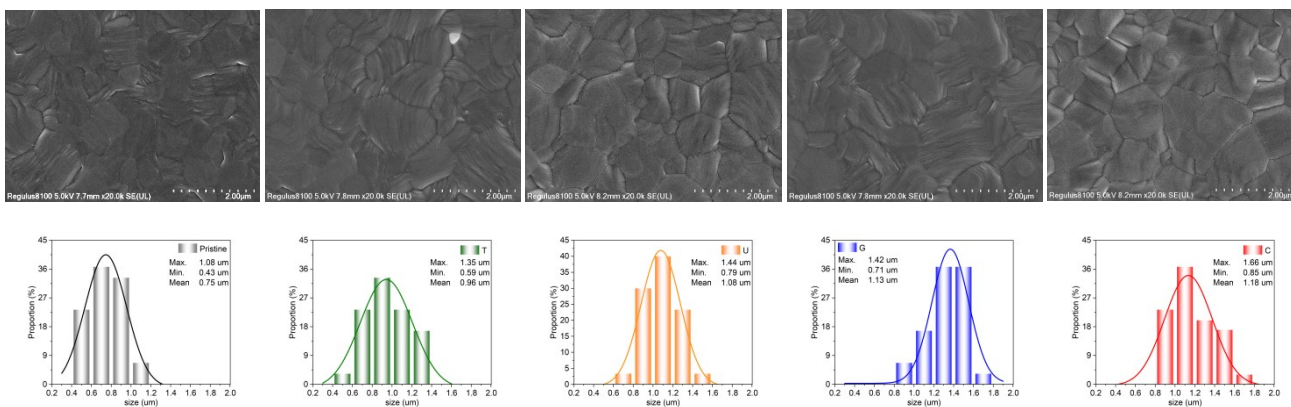
**Fig. S2** The characteristic  $J-V$  curves of pristine and C-treated PSCs under forward and reverse scanning directions. The calculation formula of hysteresis factor is  $\text{HF} = (\text{PCE}_{\text{rev}} - \text{PCE}_{\text{for}}) / \text{PCE}_{\text{rev}}$ .



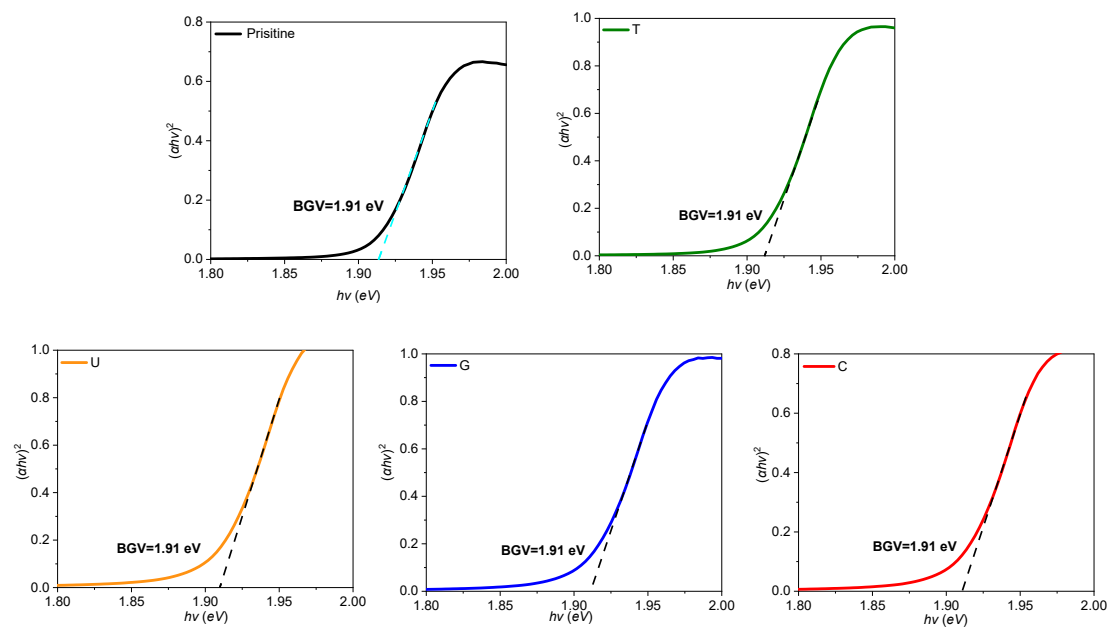
**Fig. S3** The statistical photovoltaic parameters distribution including (a)  $V_{OC}$ , (b)  $J_{SC}$  and (c) FF.



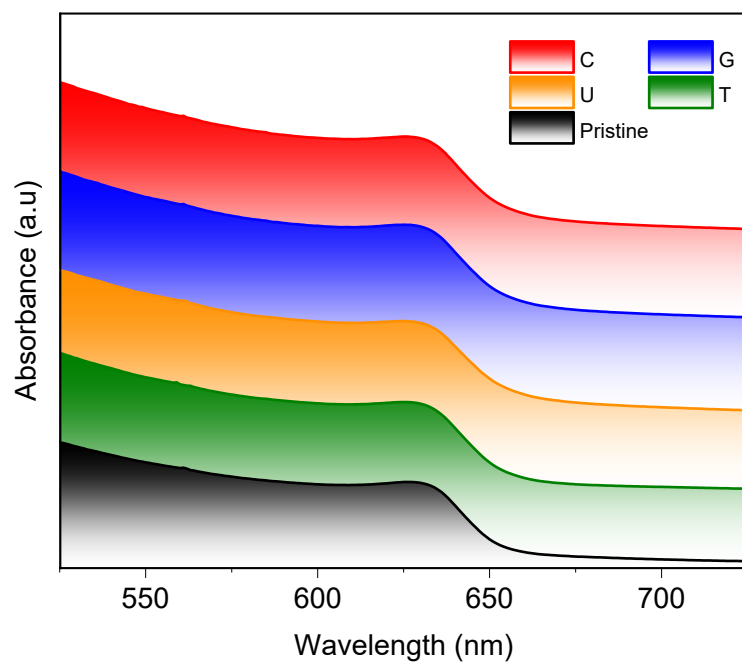
**Fig. S4**  $J_{SC}$  dependence of CsPbI<sub>2</sub>Br devices on light intensity.



**Fig. S5** Top-view SEM images and particle size distribution maps of CsPbI<sub>2</sub>Br perovskite films.

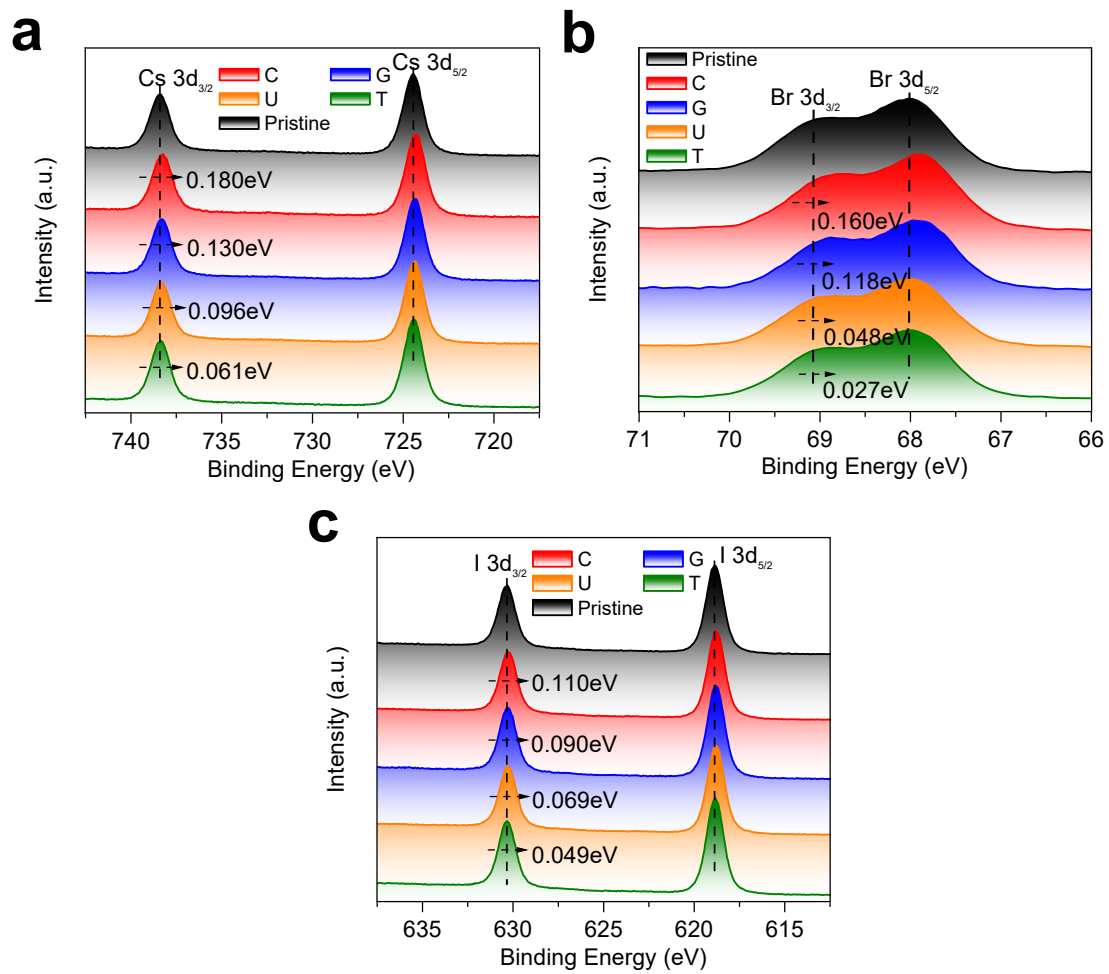


**Fig. S6** Bandgaps of CsPbI<sub>2</sub>Br perovskite films.

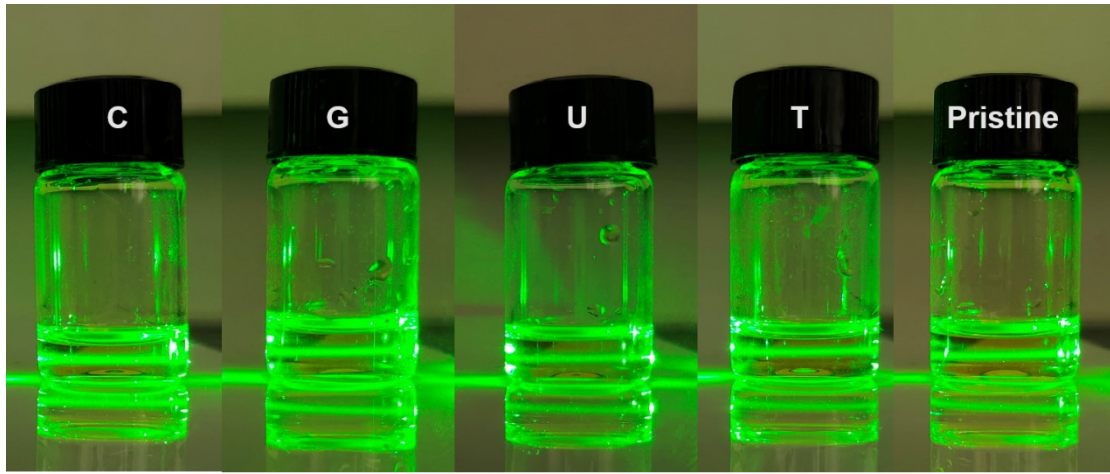


**Fig. S7** UV-vis spectra of CsPbI<sub>2</sub>Br perovskite films.

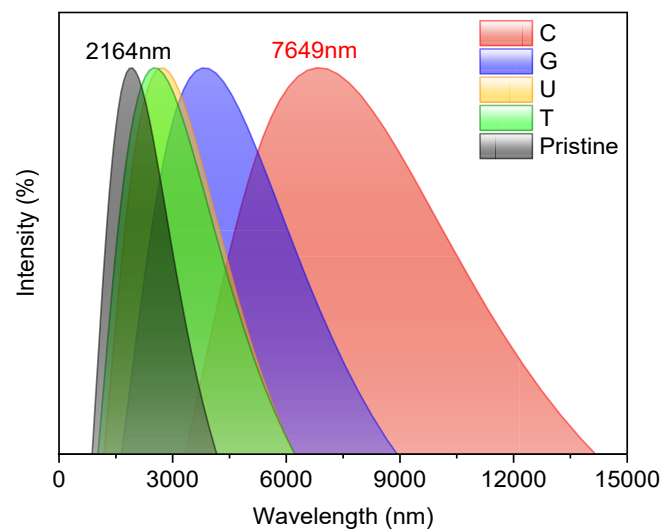




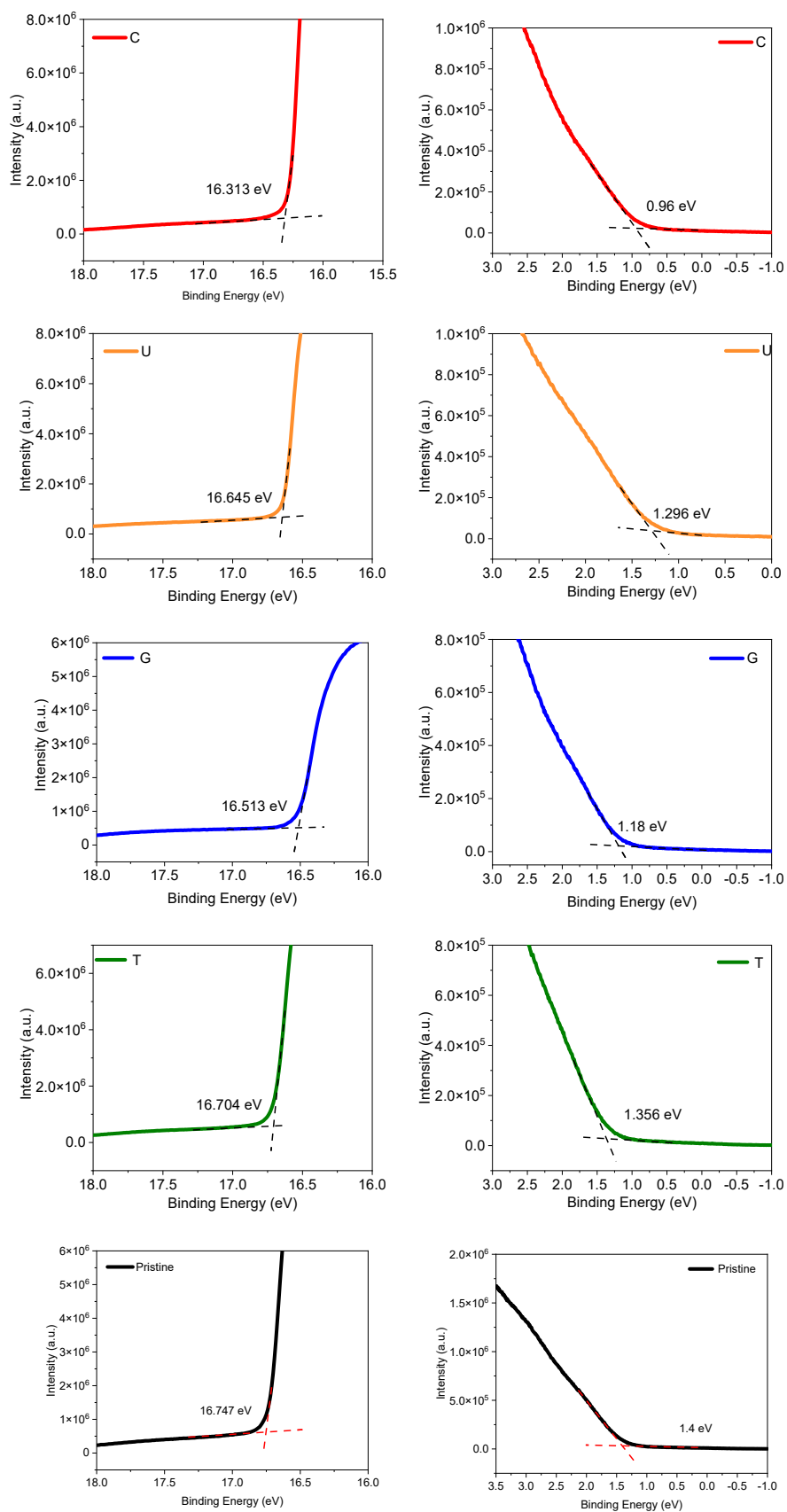
**Fig. S8** XPS spectra of (a) Cs 3d, (b) Br 3d and (c) I 3d.



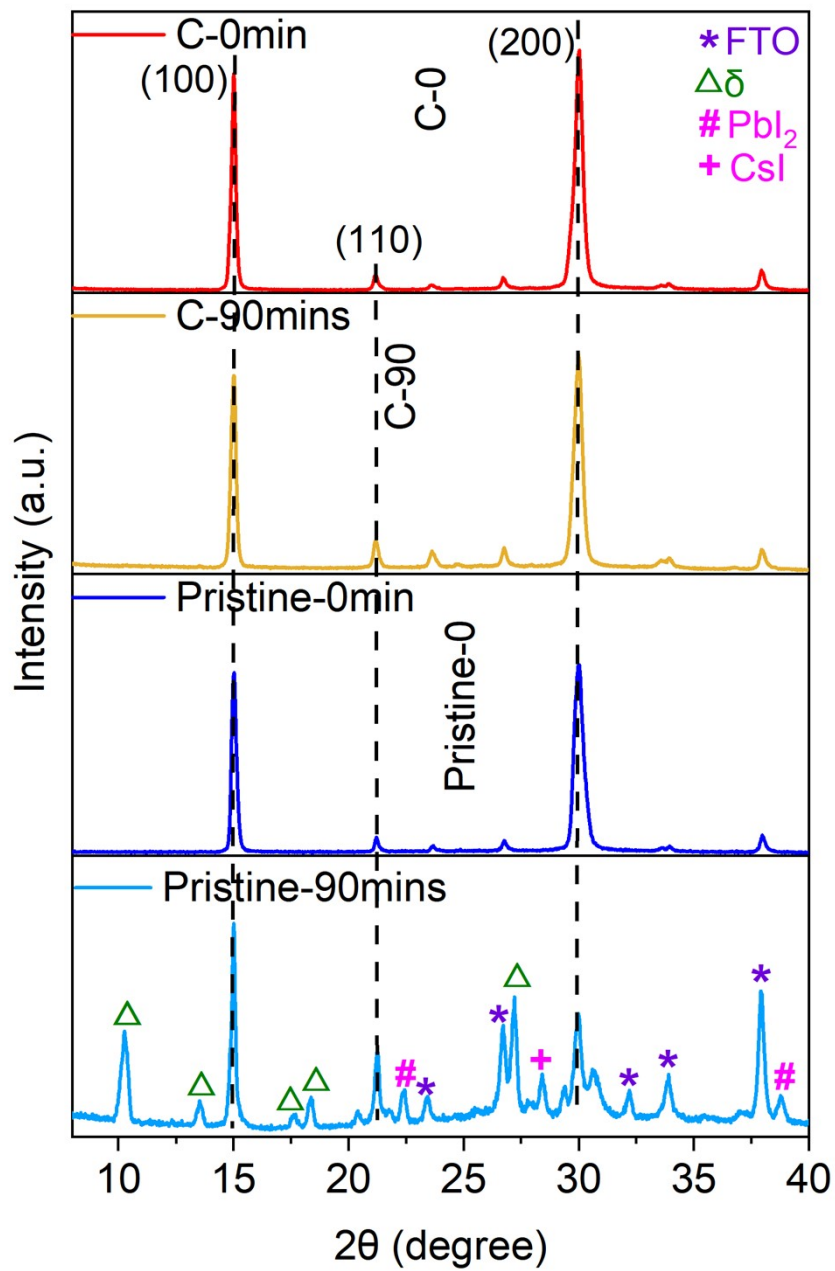
**Fig. S9** Tyndall effect of perovskite precursor solutions with different molecules.



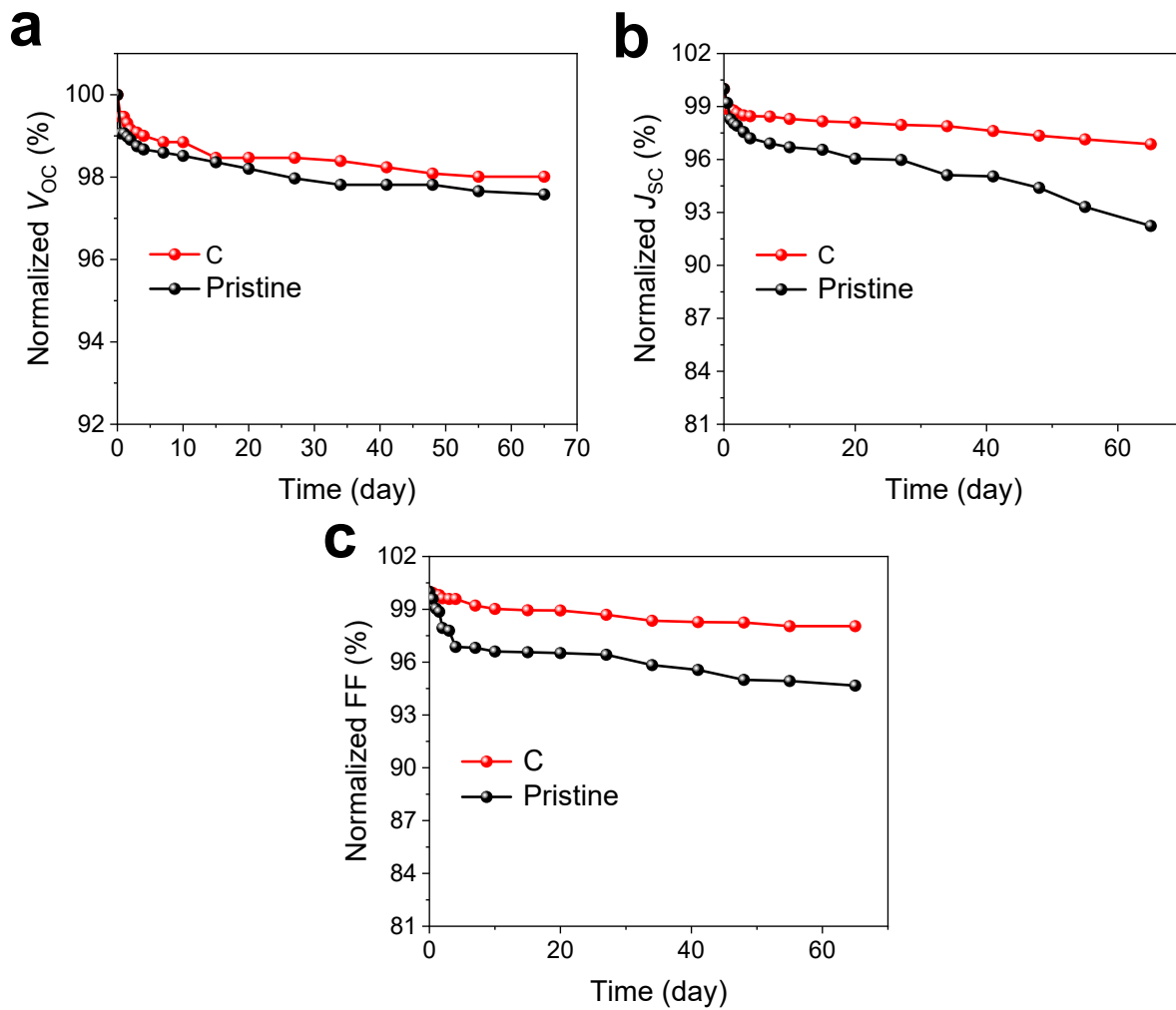
**Fig. S10** The statistical size distribution of colloids in perovskite solutions.



**Fig. S11** UPS spectra of various perovskite films.



**Fig. S12** XRD spectra of perovskite films on  $\text{TiO}_2$  substrates before and after aging treatment.



**Fig. S13** Normalized photovoltaic parameters of PSCs treated with and without Cytosine including (a)  $J_{SC}$ , (b)  $V_{OC}$  and (c) FF under 25 °C and 10% RH.

**Table S1** Photovoltaic parameters of CsPbI<sub>2</sub>Br PSCs treated by cytosine with various concentrations.

Cytosine (mg mL <sup>-1</sup> )	$V_{OC}$ (V)	$J_{SC}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
0.050	1.284	14.707	74.74	14.11
0.075	1.317	14.712	77.34	15.00
0.100	1.306	14.656	75.25	14.40

**Table S2** Photovoltaic parameters of CsPbI<sub>2</sub>Br PSCs treated by guanine with various concentrations.

Guanine (mg mL <sup>-1</sup> )	$V_{OC}$ (V)	$J_{SC}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
0.025	1.281	14.39	72.74	13.36
0.050	1.303	14.42	78.70	14.79
0.075	1.299	14.03	74.74	13.83
0.100	1.295	14.13	73.30	13.59

**Table S3** Photovoltaic parameters of CsPbI<sub>2</sub>Br PSCs treated by uracil with various concentrations.

Uracil (mg mL <sup>-1</sup> )	$V_{OC}$ (V)	$J_{SC}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
0.025	1.269	13.969	70.82	12.55
0.050	1.399	14.163	71.04	14.20
0.075	1.255	14.701	77.17	13.11
0.100	1.247	14.388	72.48	13.00

**Table S4** Photovoltaic parameters of CsPbI<sub>2</sub>Br PSCs treated by thymine with various concentrations.

Thymine (mg mL <sup>-1</sup> )	$V_{OC}$ (V)	$J_{SC}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
0.050	1.265	13.865	75.56	13.25
0.070	1.260	14.441	74.88	13.62
0.100	1.286	14.066	76.23	13.79
0.150	1.265	13.864	75.07	13.73