

Supporting Information

Structured-Crystallization for Efficient All-Inorganic Perovskite Solar Cells with High Phase Stability

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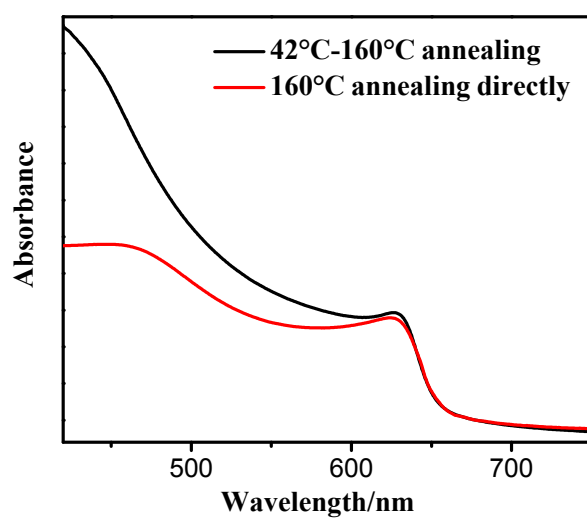


Figure S1. Absorbance spectra of CsPbI₂Br perovskite film under different annealing process.



Figure S2. Photo of ambient air with 65% RH when all-inorganic perovskite film was prepared.

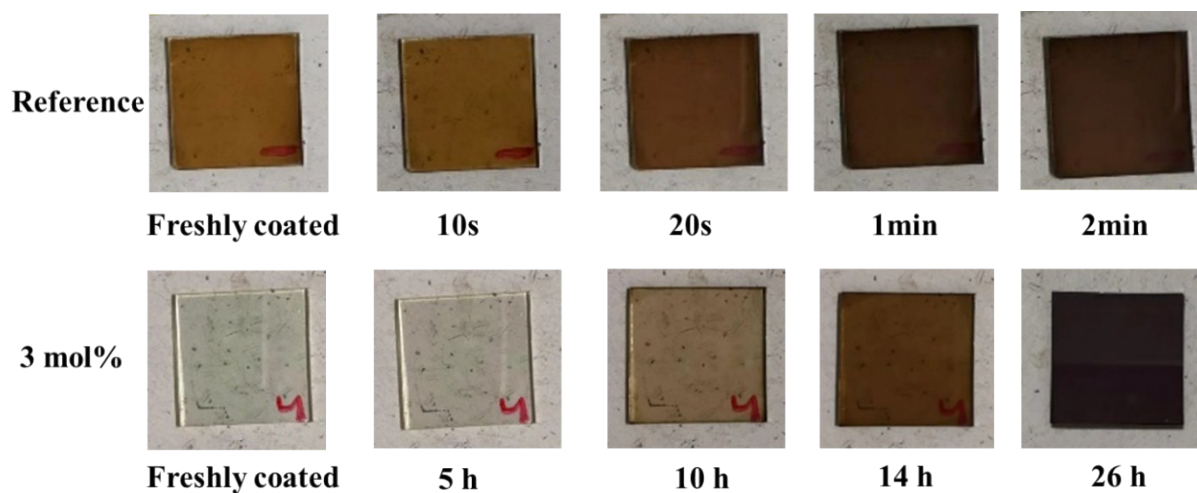


Figure S3. Optical images of CsPbI₂Br perovskite films with and without yttrium incorporation stored under ambient atmosphere at room temperature.

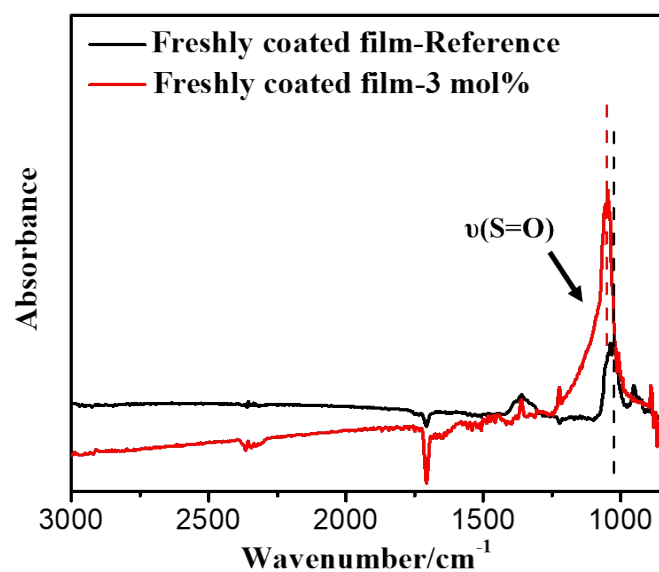


Figure S4. ATR-FTIR spectra of freshly coated CsPbI_2Br films with and without 3 mol% yttrium incorporation.

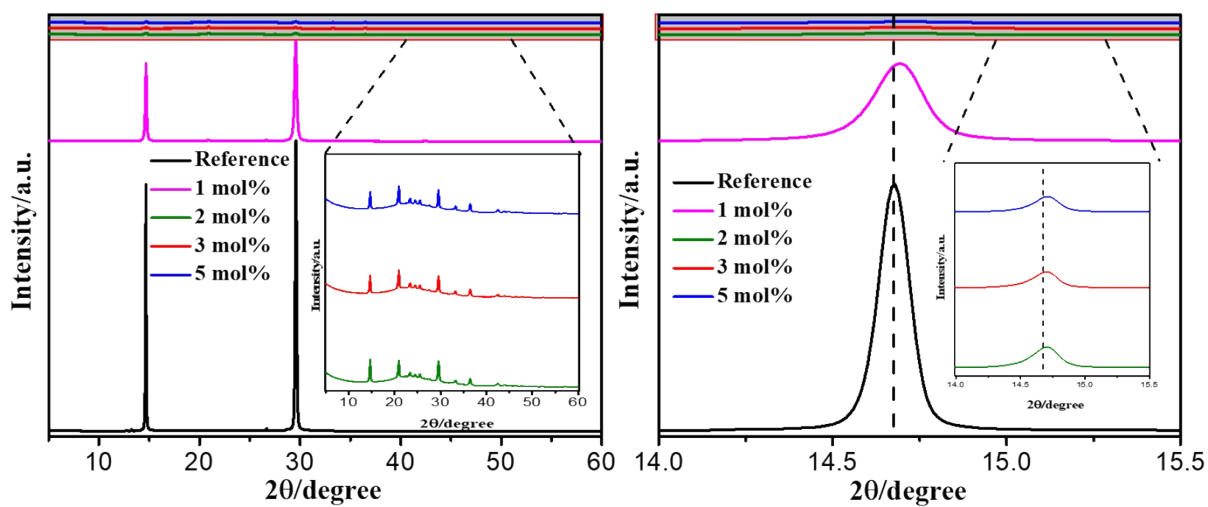


Figure S5. X-ray diffraction pattern and the corresponding magnification of the reference and yttrium-incorporated CsPbI_2Br perovskite films.

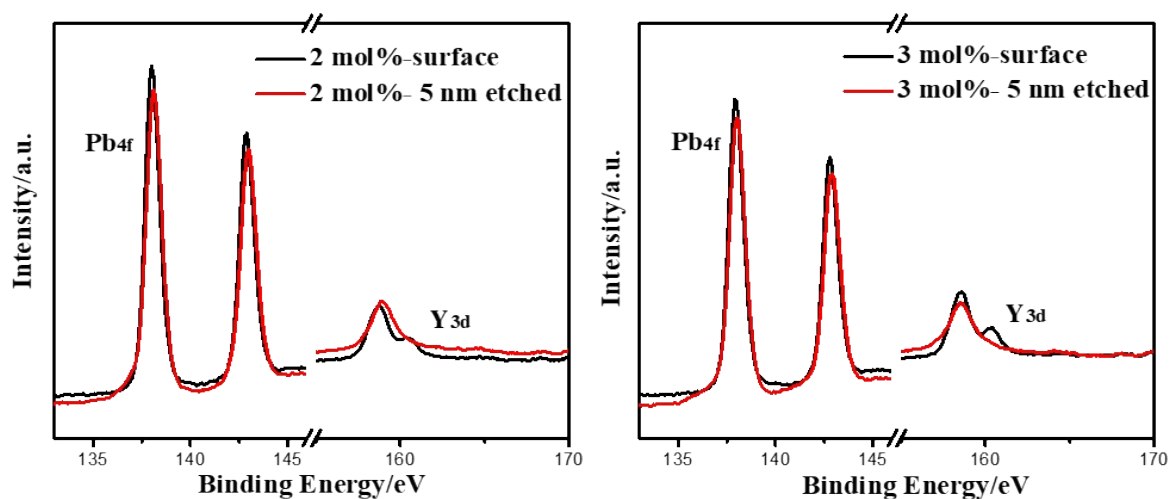


Figure S6. XPS spectra of Pb_{4f} and Y_{3d} on the surface and the depth of 5 nm by etching when 2 mol% and 3 mol% yttrium were incorporated in perovskite films.

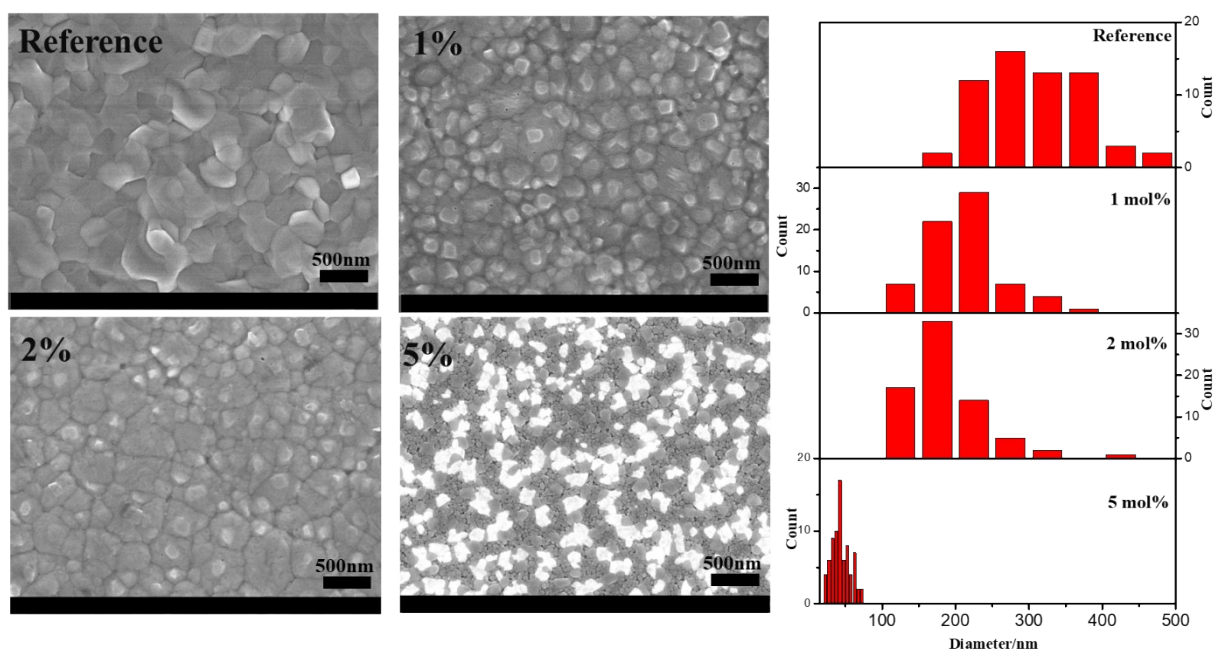


Figure S7. Top-view SEM images of CsPbI₂Br films without and with 1 mol%, 2 mol%, 5 mol% yttrium in perovskites. The corresponding column graphs of perovskite grain size statistics are shown in right.

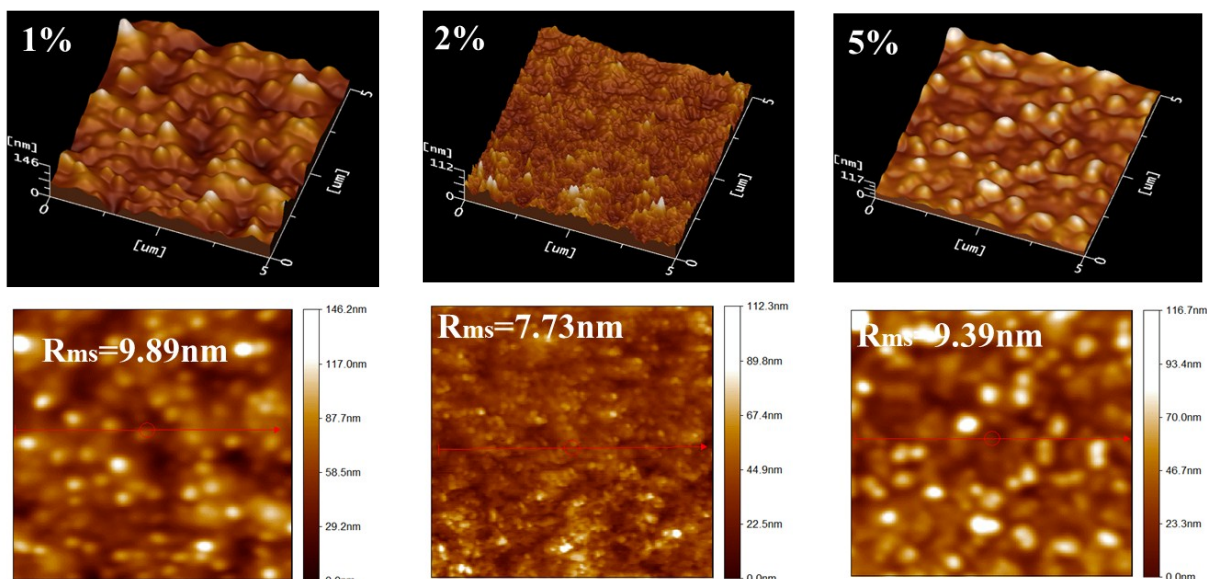


Figure S8. 3D AFM images of 1 mol%, 2 mol% and 5 mol% yttrium incorporated perovskite films and corresponding roughness shown below.

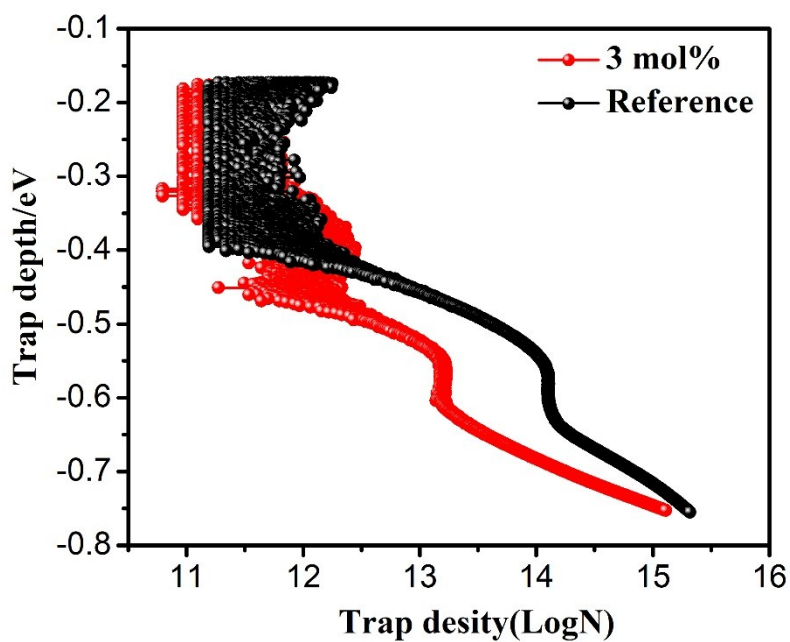


Figure S9. Trap depth as a function of trap density and trap density distribution in perovskite films with and without yttrium incorporation. The vacuum level of perovskite film was calculated according to the following equation.

$$E_{vac} = -KT \ln \frac{T^4}{\beta}$$

β represents the heating rate employed in TSC measurement, T denotes the temperature and K is the Boltzmann constant.

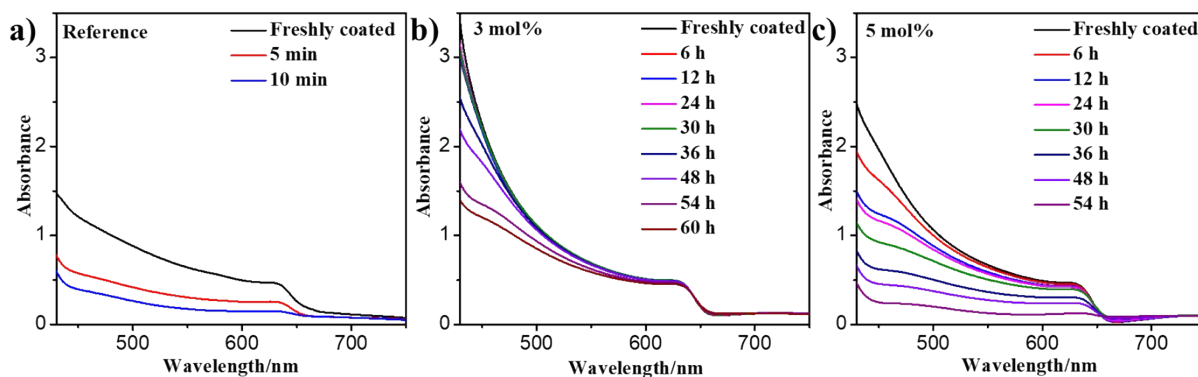


Figure S10. Evolution of absorbance spectra of a) reference, b) 3 mol% and c) 5 mol% yttrium-incorporated CsPbI_2Br films aging in humid air with 65% RH.

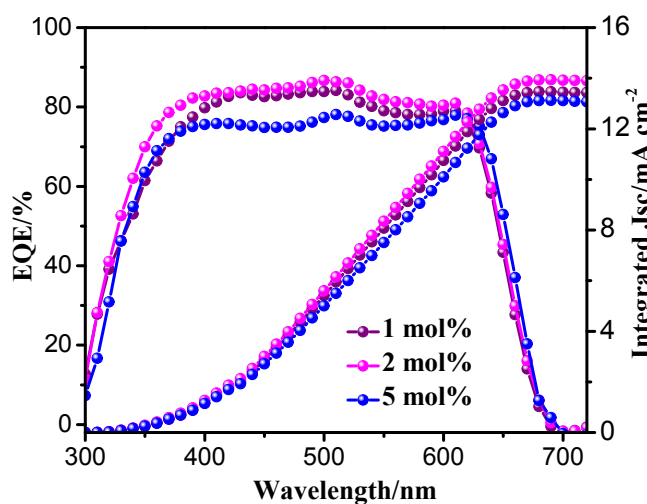


Figure S11. External quantum efficiency (EQE) spectra and integrated J_{sc} of 1 mol%, 2 mol% and 5 mol% yttrium-incorporated CsPbI_2Br PSCs.

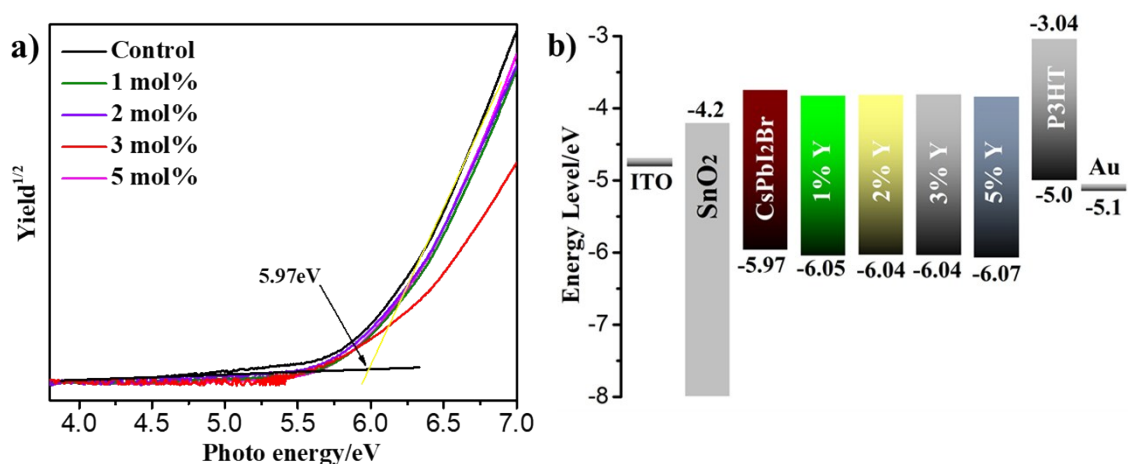


Figure S12. a) Photoelectron yield spectroscopy (PYS) spectra of CsPbI_2Br films with and without various amount of yttrium incorporation. b) Energy level diagram of perovskite device before and after yttrium incorporation.

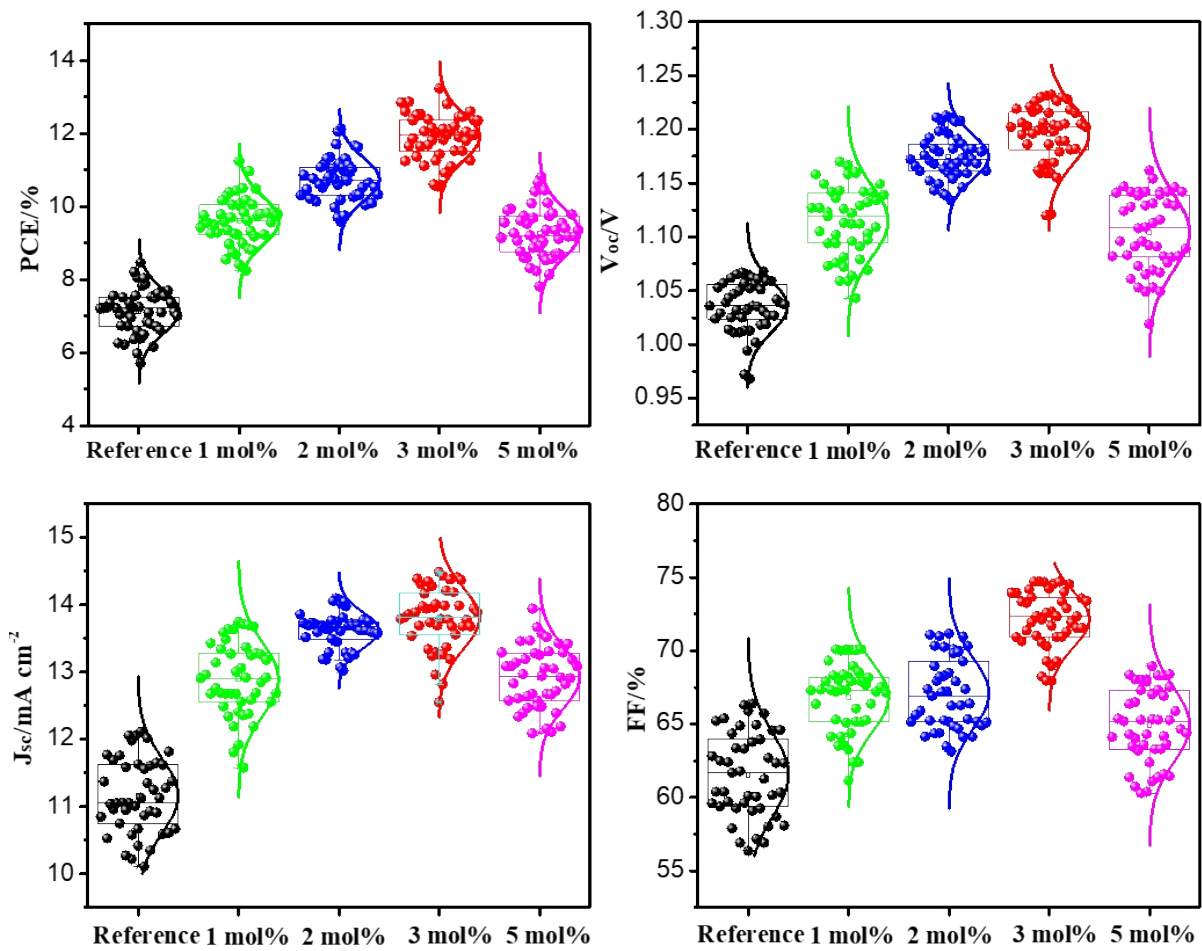


Figure S13. Statistics of the corresponding devices parameters including PCE, J_{sc} , V_{oc} and FF.

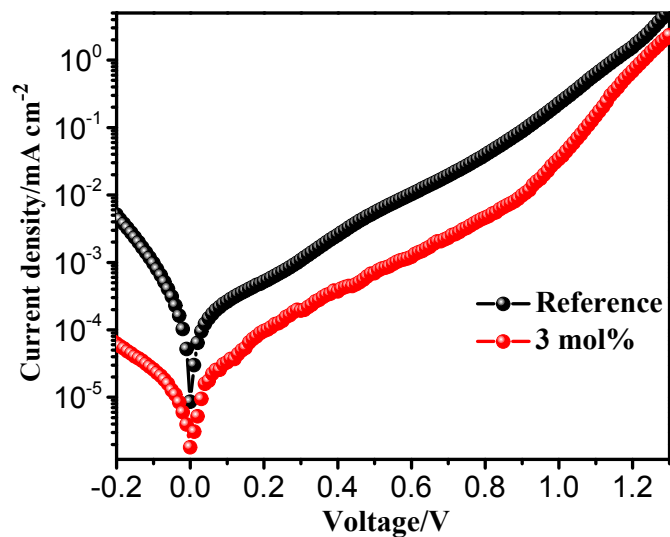


Figure S14. Dark J-V characteristics on a semilog scale based on CsPbI₂Br PSCs with and without 3 mol% yttrium incorporation.

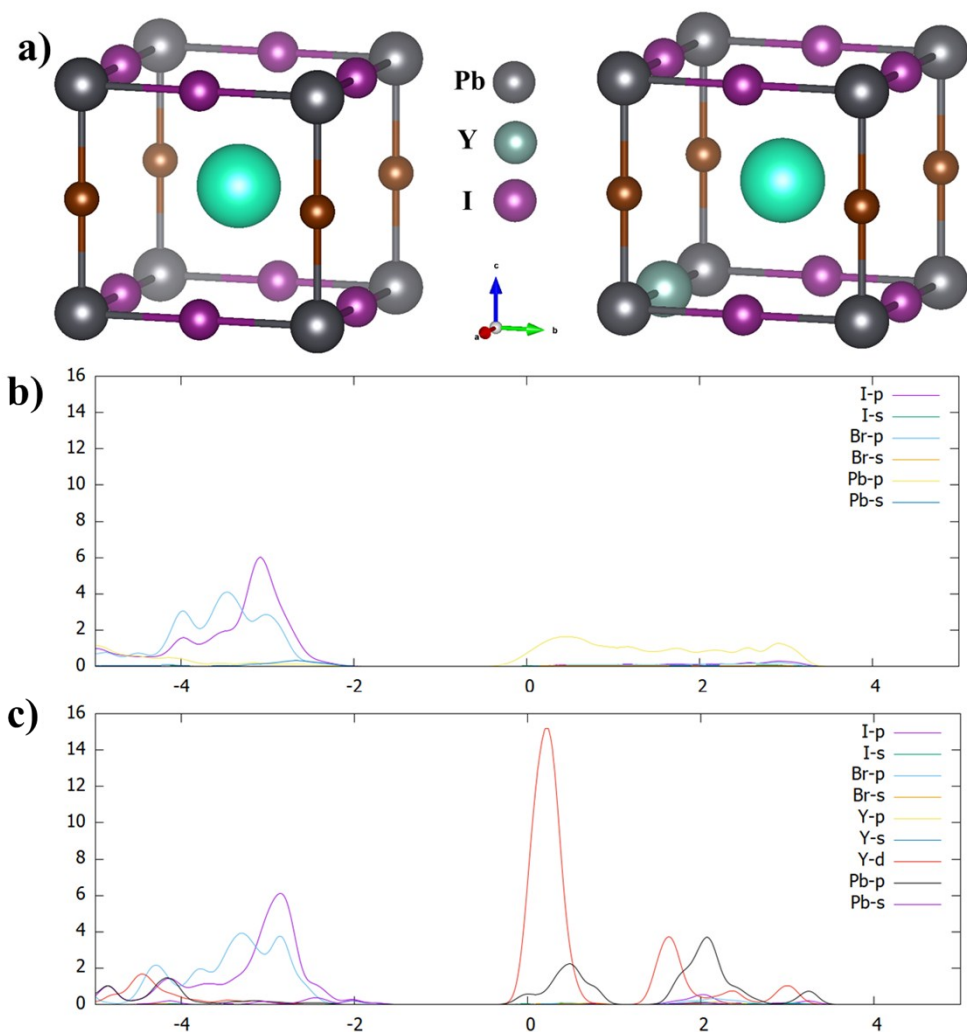


Figure S15. a) Geometric structures of CsPbI₂Br and CsPb_{0.875}Y_{0.125}I₂Br perovskites. Calculated DOS for b) the CsPbI₂Br perovskite and c) CsPb_{0.875}Y_{0.125}I₂Br perovskite.

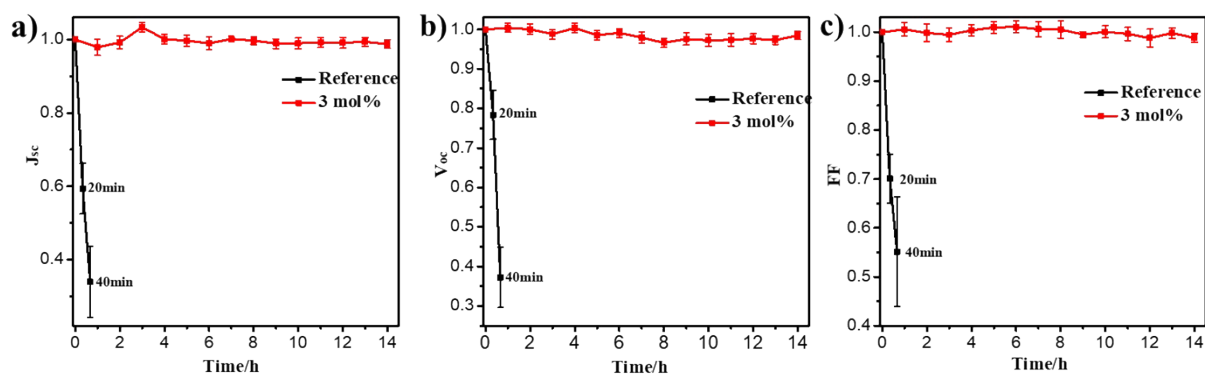


Figure S16. Stability tests for normalized a) J_{sc} , b) V_{oc} and c) FF of the reference and 3 mol% yttrium-incorporated CsPbI₂Br PSCs without encapsulation in ambient air with 65% RH.

Table S1. Summary of 2 mol% and 3 mol% yttrium-incorporated CsPbI₂Br chemical composition including the surface and 5 nm depth of perovskite films.

		J _{sc} (mA cm ⁻²)	V _{oc} (V)	FF (%)	PCE (%)	Hysteresis Index (%)
Reference	F	12.02	1.047	56.07	7.05	20
	R	12.11	1.065	65.89	8.46	
3 mol%	F	14.44	1.234	74.01	13.19	4
	R	14.49	1.232	74.23	13.25	

Table S2. Parameters of the photovoltaic parameters of CsPbI₂Br and CsPb_{0.97}Y_{0.03}I₂Br PSCs at forward (F) and reverse (R) scans.

		Y _{3d}	Pb _{4f}	Area ratio(Y _{3d} /Pb _{4f})
2%	surface	14169.4	70737.5	0.2
	etching	13449.9	72456.0	0.19
3%	surface	16129.8	61469.9	0.26
	etching	13954.5	59647.7	0.23

Table S3. Summary of parameters fitted from TRPL spectra using the double-exponential equation.

perovskite	τ ₁ (ns)	τ ₂ (ns)
CsPbI ₂ Br	0.26	0.81
CsPb _{0.97} Y _{0.03} I ₂ Br	3.98	7.85

