Supporting Information

Bulk and Surface Defect Manipulation of the ZnO ETL for All-inorganic $CsPbBr_3$ Perovskite Solar Cells

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This appendix includes:

Figures S1~S13

Tables S1~S8

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Figures S1-S13

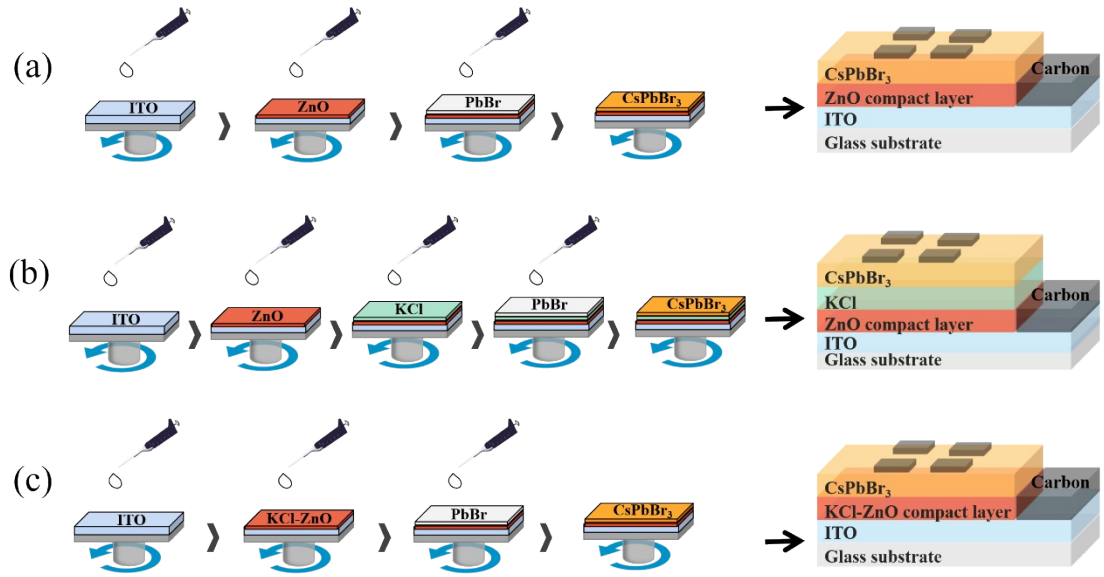

Figure S1. Schematic diagram of the device preparation process of ZnO thin films prepared by different treatment methods: (a) ITO/O-ZnO/$CsPbBr_3$/Carbon; (b) ITO/M-ZnO/$CsPbBr_3$/Carbon; (c) ITO/D-ZnO/$CsPbBr_3$/Carbon.

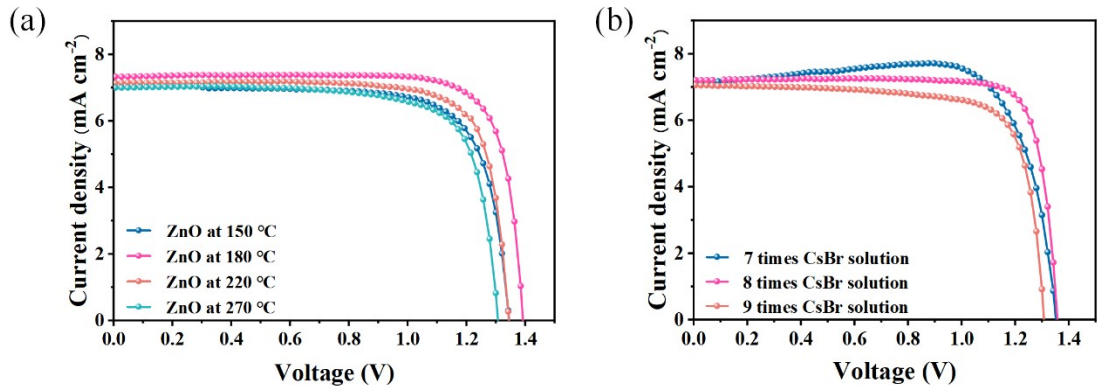

Figure S2. Test diagram of J-V characteristic curve under different conditions: (a) different annealing temperatures of ZnO ETL; (b) CsBr solution spin coating times.

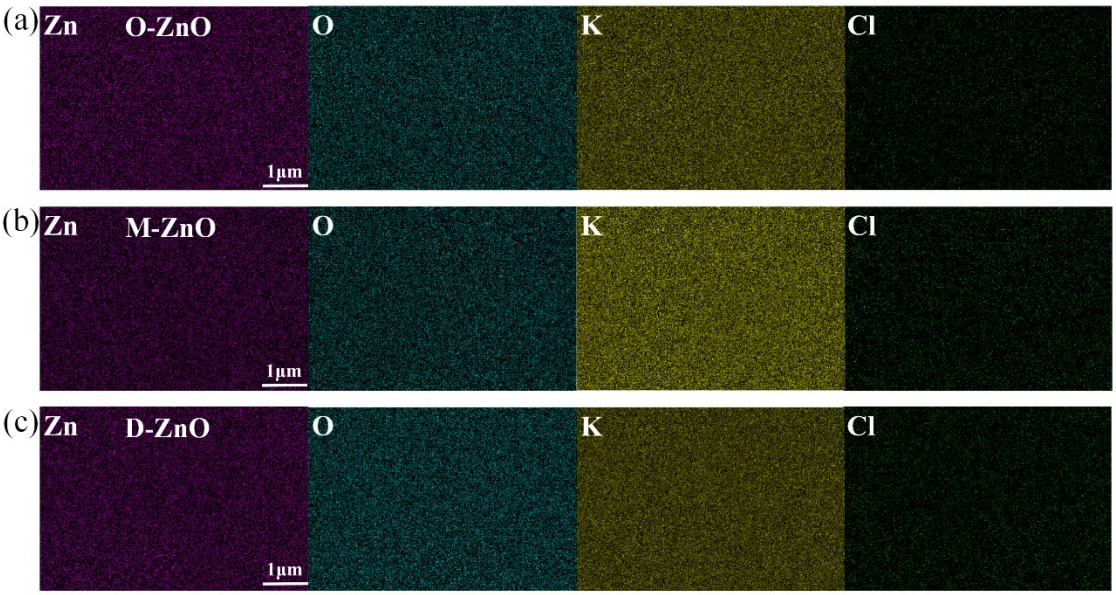

Figure S3. EDS test diagram of different ZnO films: (a) O-ZnO; (b) M-ZnO; (c) D-ZnO.

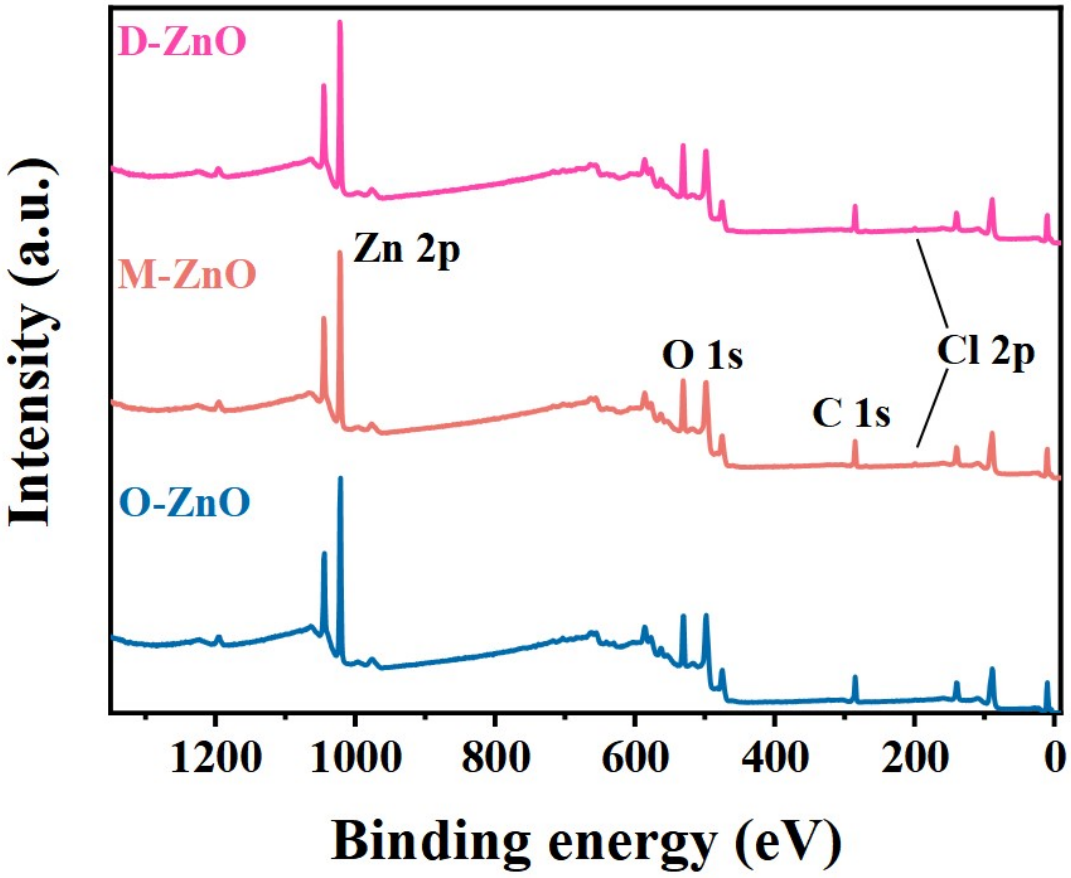

Figure S4. Full XPS spectra of different ZnO films.

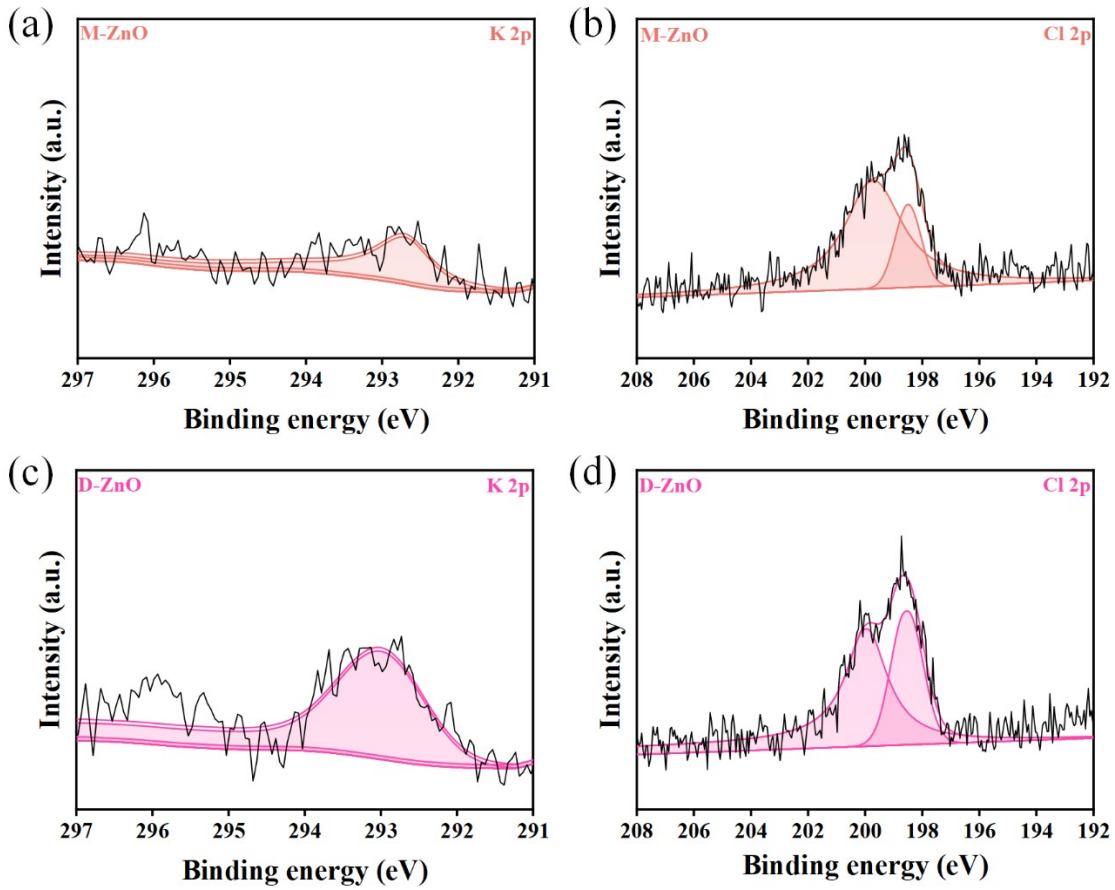

Figure S5. XPS test spectra of M-ZnO thin films: (a) K 2p; (b) Cl 2p. XPS test spectra of D-ZnO thin films: (c) K 2p; (d) Cl 2p.

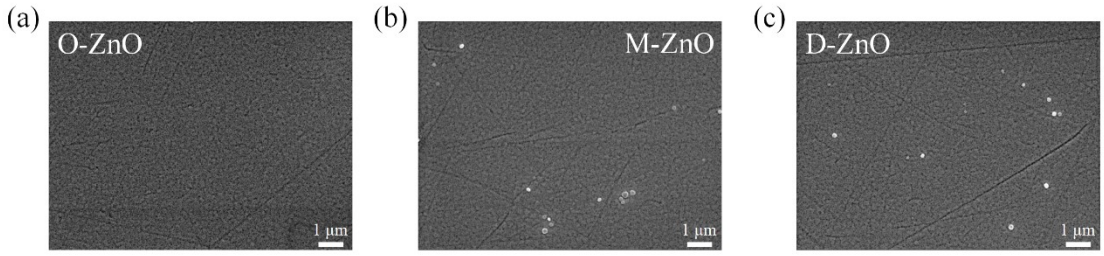

Figure S6. SEM images of different ZnO films: (a) O-ZnO; (b) M-ZnO (c) D-ZnO.

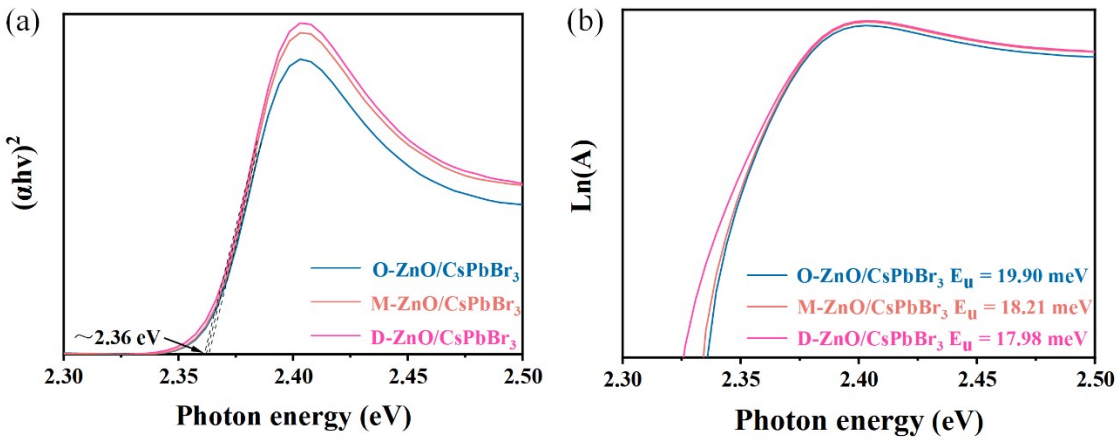

Figure S7. Curves of $CsPbBr_3$ films on different ZnO ETL: (a) Tauc curve; (b) Urbach energy.

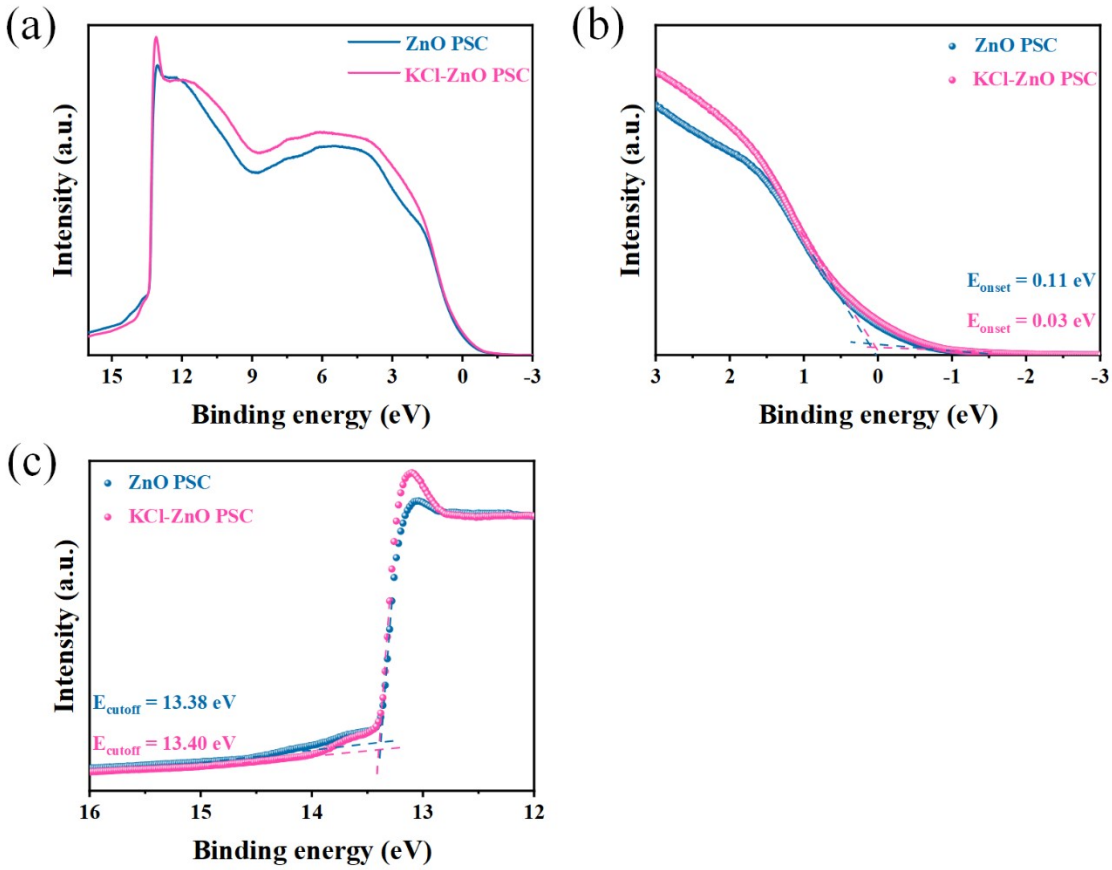

Figure S8. UPS curves of the original ZnO PSC and KCl-ZnO PSC: (a) Full spectrum; (b) Onset; (c) Cutoff regions.

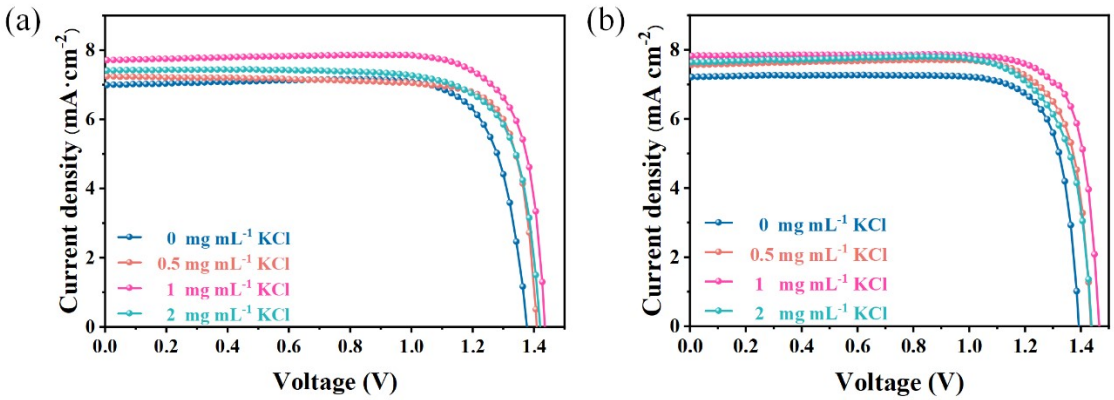

Figure S9. Test diagram of J-V characteristic curve under different conditions: (a) KCl modification; (b) KCl doping.

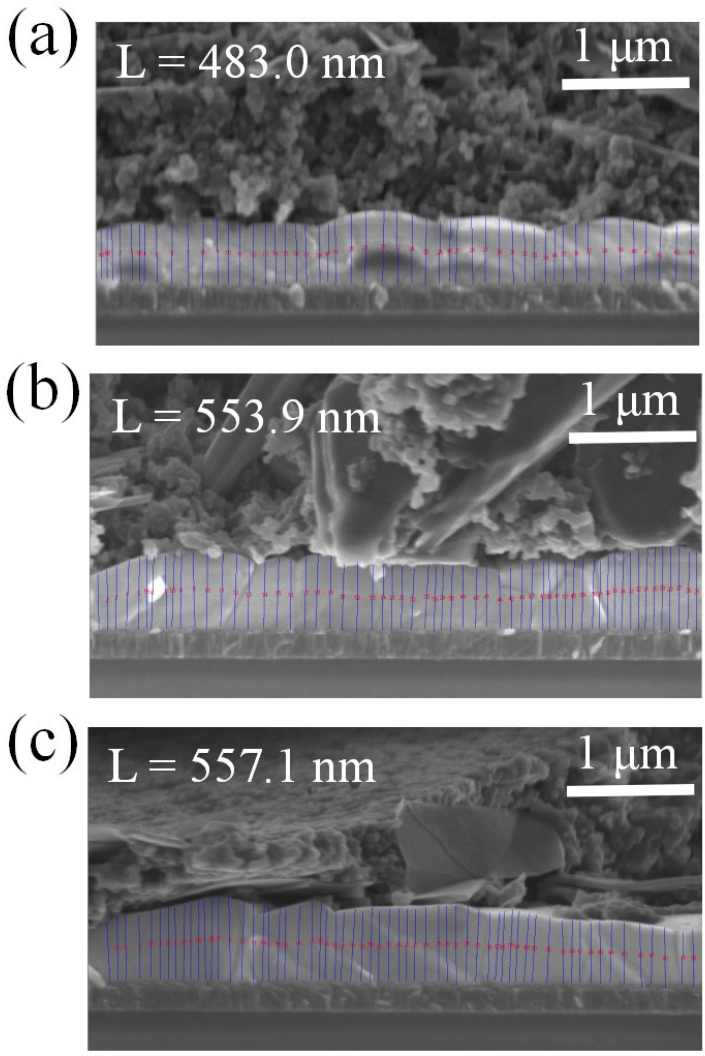

Figure S10 Calculation of $CsPbBr_3$ PVK thickness by the cross-sectional SEM images and the Nano Measure 1.2 software.

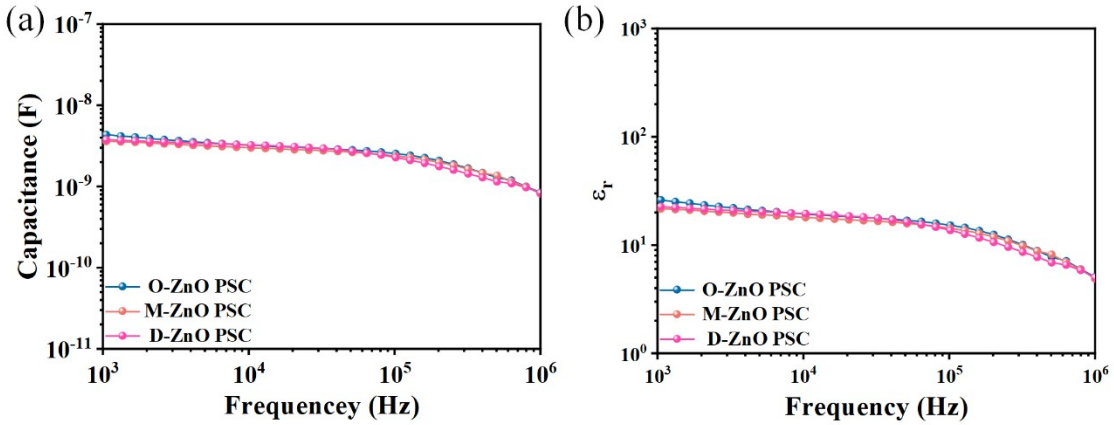

Figure S11. (a) Capacitance versus frequency (C-f) curve; (b) the frequency-dependent dielectric constant (ε_r-f).

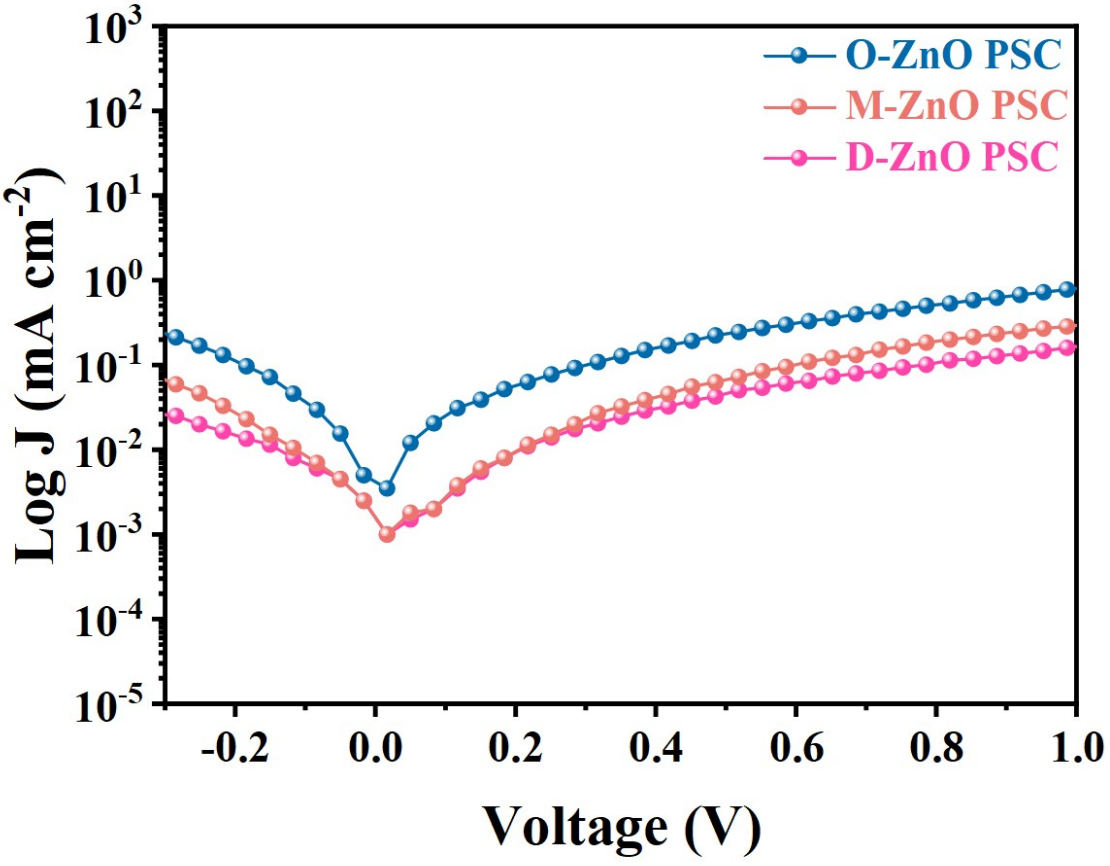

Figure S12. The dark J-V curves of various $CsPbBr_3$ PSCs.

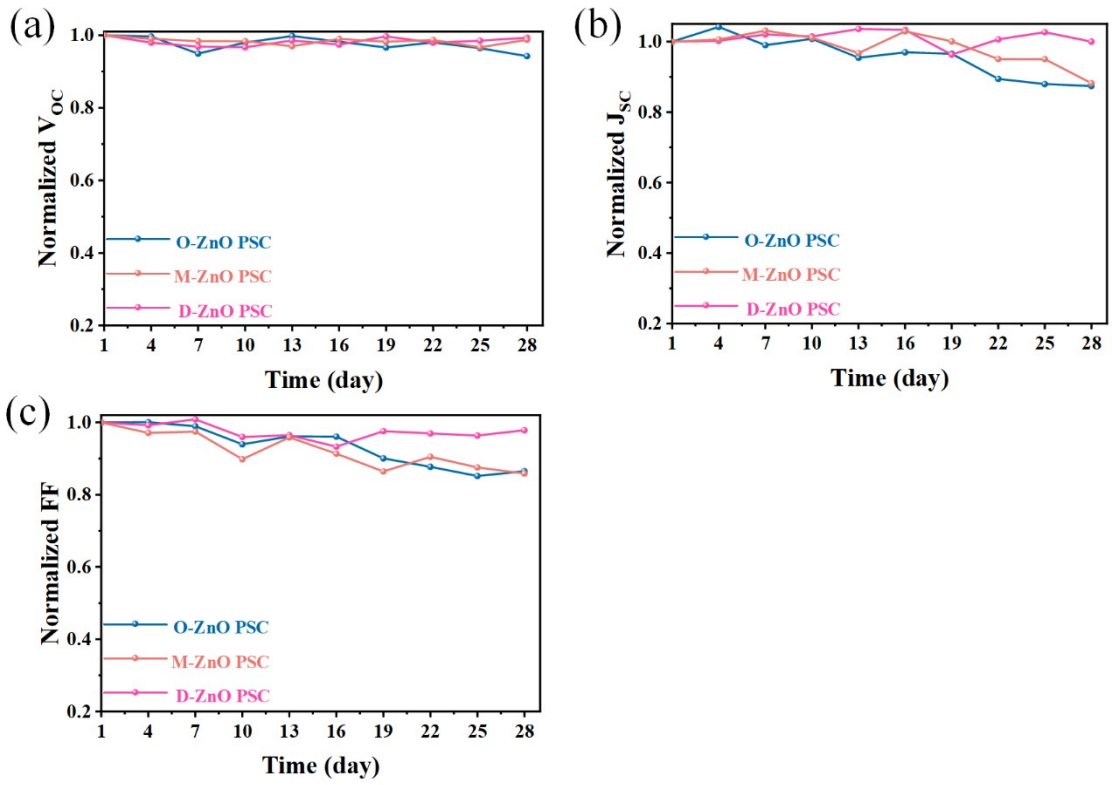

Figure S13. Device photovoltaic parameter stability test curve: (a) V_{OC}; (b) J_{SC}; (c) FF.

Table S1-S8

Table S1. Photovoltaic parameters of the $CsPbBr_3$ PSCs at different annealing temperatures of ZnO ETL.

Annealing temperature (°C)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
150	1.34	6.98	75.36	7.05
180	1.39	7.30	80.45	8.16
220	1.34	7.12	78.21	7.46
270	1.30	6.99	75.66	6.88

Table S2. Photovoltaic parameters of the $CsPbBr_3$ PSCs with different spin coating times of CsBr solution.

Times of spin coating	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
7	1.35	7.07	80.63	7.70
8	1.36	7.19	82.74	8.09
9	1.31	7.07	76.05	7.04

Table S3. Atomic percentage of element distribution in different ZnO films.

Sample	Zn (%)	O (%)	K (%)	Cl (%)
O-ZnO	11.38	68.70	19.90	0.01
M-ZnO	11.11	68.11	20.53	0.25
D-ZnO	10.53	68.69	20.54	0.23

Table S4. TRPL curve parameters of $CsPbBr_3$ films on different ZnO ETL.

Films	τ_{ave} (ns)	τ_1 (ns)	τ_2 (ns)	A_1 (%)	A_2 (%)
O-ZnO/$CsPbBr_3$	7.54	2.64	14.57	42.50	44.02
M-ZnO/$CsPbBr_3$	3.63	1.57	7.22	62.80	36.61
D-ZnO/$CsPbBr_3$	1.97	0.74	5.40	63.39	27.83

Table S5. Calculation results of energy levels in different devices.

Films	$E_{cut\text{-}off}$ (eV)	$E_{on\text{-}set}$ (eV)	W_F (eV)	E_{VB} (eV)	E_g (eV)	E_{CB} (eV)
ZnO	13.38	0.11	7.84	-7.93	3.3	-4.63
KCl-ZnO	13.40	0.03	7.82	-7.83	3.3	-4.53

Table S6. Photovoltaic parameters of $CsPbBr_3$ PSCs modified by ZnO ETL with different concentrations of KCl.

Concentration (mg mL^{-1})	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
0.00	1.38	6.99	79.47	7.67
0.50	1.41	7.25	80.36	8.21
1.00	1.44	7.70	80.36	8.91
2.00	1.42	7.42	76.66	8.08

Table S7. Photovoltaic parameters of $CsPbBr_3$ PSCs doped with ZnO ETL at different concentrations of KCl.

Concentration (mg mL^{-1})	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
0.00	1.39	7.19	80.45	8.04
0.50	1.43	7.55	80.35	8.67
1.00	1.46	7.82	80.73	9.22
2.00	1.43	7.61	77.53	8.44

Table S8. Photovoltaic parameters of $CsPbBr_3$ PSCs of ZnO ETL with different treatment methods**.**

Sample	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
O-ZnO PSC	1.39	7.23	80.45	8.08
M-ZnO PSC	1.44	7.70	80.36	8.91
D-ZnO PSC	1.46	7.82	80.73	9.22