Supporting Information

Molecular Engineering with CuanCl for Effectual Optimization of Defective Interface for Wide-Bandgap Perovskite Solar Cells

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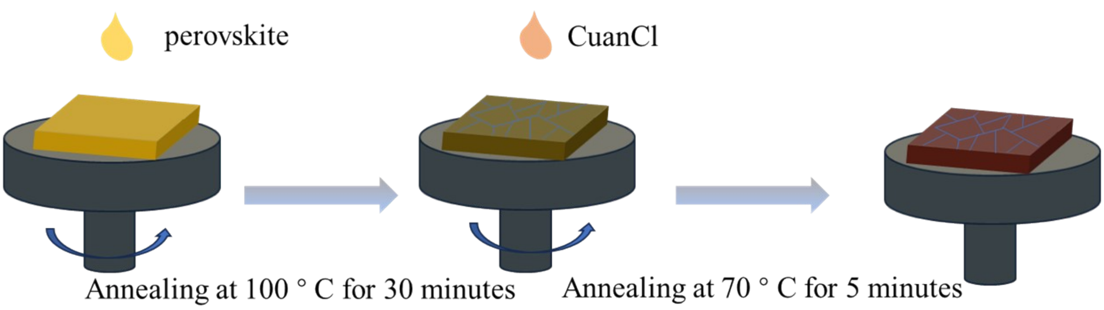

Fig. S1 Schematic representation of the process for post-treatment of perovskite films with CuanCl.

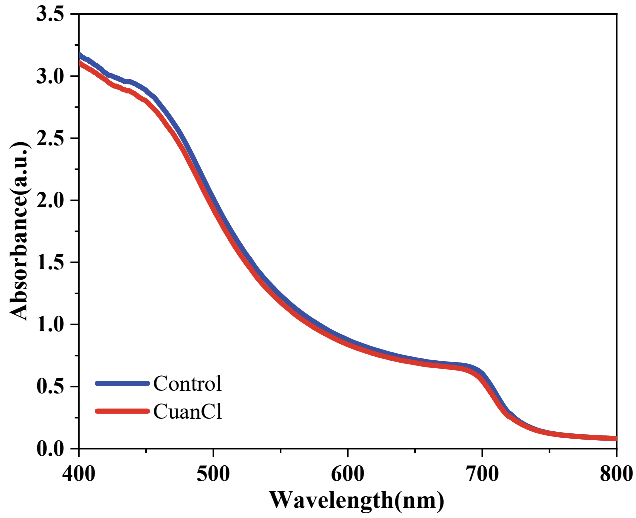

Fig. S2 UV–Vis spectra of the perovskite prepared with and without CuanCl treatment.

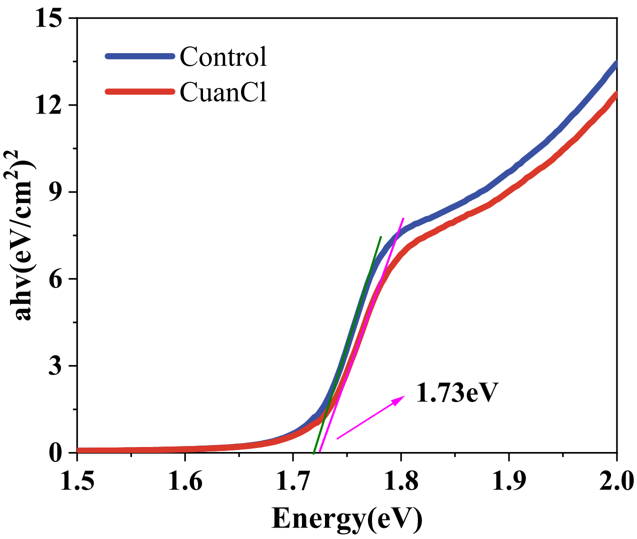

Fig. S3 Tauc plot calculated from the UV-vis.

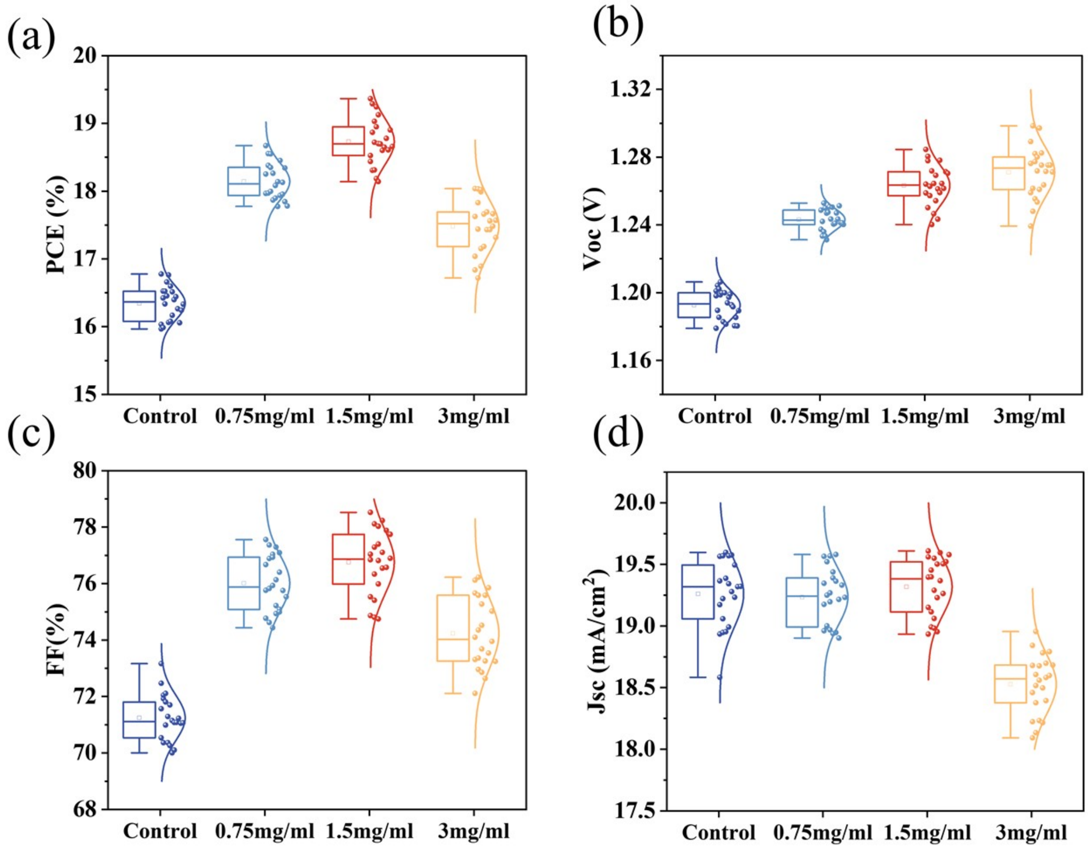

Fig. S4 The photovoltaic parameters of WBG PSCs: (a) PCE, (b) V_{OC}, (c) FF, and (d) Jsc, extracted from J–V measurements of PSCs based on different CuanCl concentrations treatment.

Table S1 The fitting parameters of the TRPL spectra of the perovskite thin films.

Sample	A_1 (%)	τ_1 (ns)	A_2 (%)	τ_2 (ns)	τ_{ave} (ns)
Control	100.40	10.40	25.25	149.29	119.16
CuanCl	35.10	80.43	24.83	600.67	517.87

Table S2 Comparing the $J_{SC, EQE}$ and $J_{SC, JV}$ between the control device and the CuanCl-treated device.

Sample	$J_{SC, JV}$[mA cm^{-2}]	$J_{SC, EQE}$ [mA cm^{-2}]	Deviation percentage[%]
Control	19.56	18.98	3.0
CuanCl	19.60	18.67	4.7

Table S3 Statistical summary of the photovoltaic parameters for wide-bandgap perovskite solar cells with reported Eg>1.7 eV in the literature.

Eg [eV]	Perovskite	V_{OC} [eV]	J_{SC} [mA cm^{-1}]	FF [%]	PCE [%]	V_{loss} [V]	REF
1.8	$FA_{0.9}Cs_{0.1}Pb(I_{0.6}Br_{0.4})_3$	1.26	18.07	83.44	18.92	0.54	1
1.77	$FA_{0.8}Cs_{0.2}Pb(I_{0.6}Br_{0.4})_3$	1.29	17.54	82.61	18.63	0.48	2
1.76	$FA_{0.8}Cs_{0.2}Pb(I_{0.6}Br_{0.4})_3$	1.26	18.5	76.5	17.8	0.50	3
1.74	$FA_{0.83}Cs_{0.12}MA_{0.05}Pb(I_{0.6}Br_{0.4})_3$	1.25	19.8	79.8	20.1	0.49	4
1.77	$FA_{0.8}Cs_{0.2}Pb(I_{0.6}Br_{0.4})_3$	1.25	18.79	83.70	19.66	0.52	5
1.75	$FA_{0.8}$ $Cs_{0.2}Pb(I_{0.7}Br_{0.3})_3$	1.28	18.85	78.5	18.85	0.47	6
1.7	$FA_{0.85}Cs_{0.15}Pb(I_{0.7}Br_{0.3})_3$	1.20	20.24	80.4	18.91	0.50	7
1.78	$(FA_{0.79}MA_{0.16}Cs_{0.05})_{0.95}$ $Rb_{0.05}Pb(I_{0.6}Br^{0.4})_3$	1.19	18.53	80.3	17.71	0.59	8
1.74	$FA_{0.83}Cs_{0.17}Pb(I_{0.6}Br_{0.4})_3$	1.28	19.1	76.6	19.1	0.46	9
1.73	$FA_{0.8}$ $Cs_{0.2}Pb(I_{0.7}Br_{0.3})_3$	1.25	19.48	78.9	19.07	0.48	10
1.75	$FA_{0.8}$ $Cs_{0.2}Pb(I_{0.7}Br_{0.3})_3$	1.24	17.92	81.9	18.19	0.51	11
1.74	$FA_{0.83}Cs_{0.17}Pb(I_{0.6}Br_{0.4})_3$	1.20	19.84	78	18.51	0.54	12
1.73	$FA_{0.8}$ $Cs_{0.2}Pb(I_{0.7}Br_{0.3})_3$	1.27	19.60	77.28	19.36	0.46	This work

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