

Supporting Information for

## Efficient Semi-Transparent Wide-Bandgap Perovskite Solar Cells Enabled by Pure-Chloride 2D-Perovskite Passivation

Liu Yang<sup>1, #</sup>, Yongbin Jin<sup>1, #</sup>, Zheng Fang<sup>2, #</sup>, Jinyan Zhang<sup>3</sup>, Ziang Nan<sup>4</sup>, Lingfang Zheng<sup>1</sup>, Huihu Zhuang<sup>3</sup>, Qinghua Zeng<sup>3</sup>, Kaikai Liu<sup>1</sup>, Bingru Deng<sup>1</sup>, Huiping Feng<sup>1</sup>, Yujie Luo<sup>1</sup>, Chengbo Tian<sup>1</sup>, Changcai Cui<sup>2</sup>, Liqiang Xie<sup>1, \*</sup>, Xipeng Xu<sup>2, \*</sup>, and Zhanhua Wei<sup>1, \*</sup>

<sup>1</sup>Xiamen Key Laboratory of Optoelectronic Materials and Advanced Manufacturing, Institute of Luminescent Materials and Information Displays, College of Materials Science and Engineering, Huaqiao University, Xiamen 361021, P. R. China

<sup>2</sup>MOE Engineering Research Center for Brittle Materials Machining, Institute of Manufacturing Engineering, College of Mechanical Engineering and Automation, Huaqiao University, Xiamen 361021, P. R. China

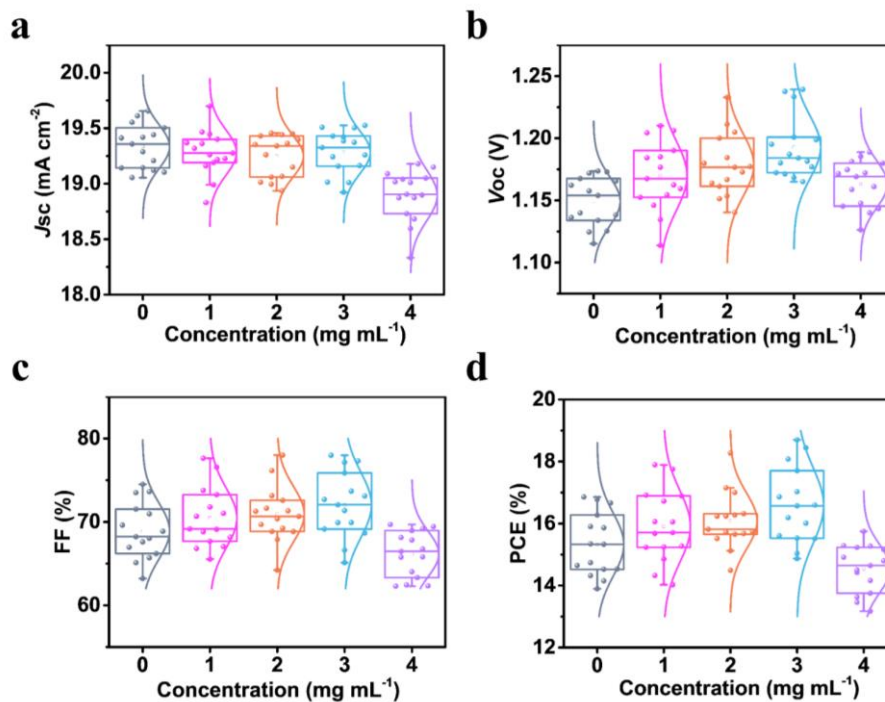
<sup>3</sup>Gold Stone (Fujian) Energy Company Limited, Quanzhou 362005, P. R. China

<sup>4</sup>Collaborative Innovation Center of Chemistry for Energy Materials, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China

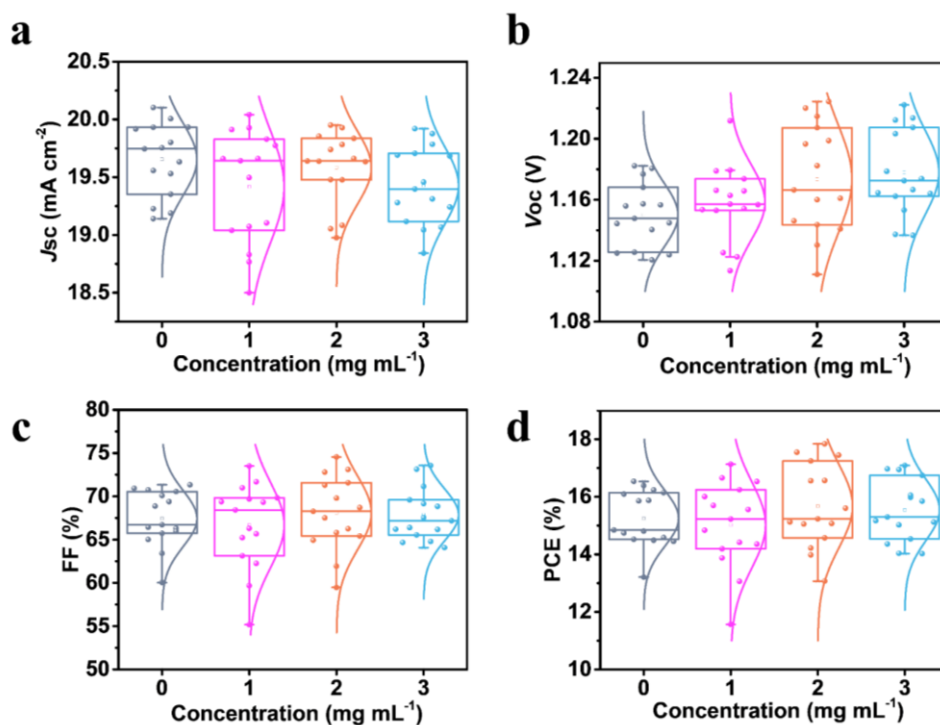
# Liu Yang, Yongbin Jin and Zheng Fang contributed equally to this work.

\*Corresponding authors. E-mail: [lqxie@hqu.edu.cn](mailto:lqxie@hqu.edu.cn) (Liqiang Xie); [xpxu@hqu.edu.cn](mailto:xpxu@hqu.edu.cn) (Xipeng Xu); [weizhanhua@hqu.edu.cn](mailto:weizhanhua@hqu.edu.cn) (Zhanhua Wei)

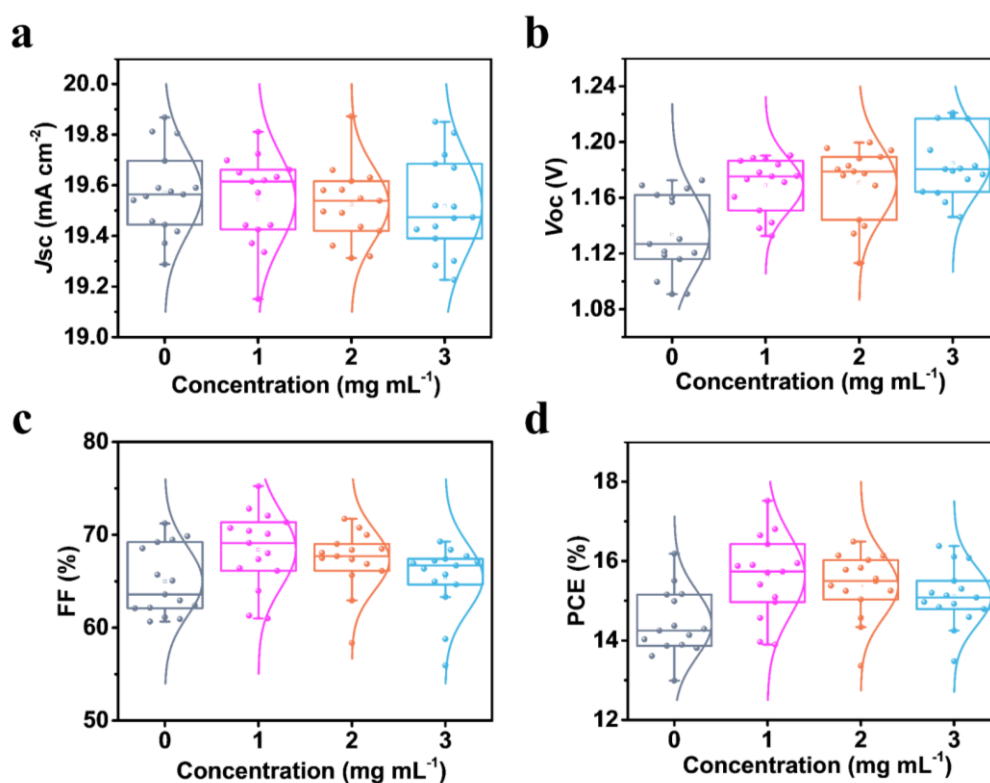
### Supplementary Figures and Tables



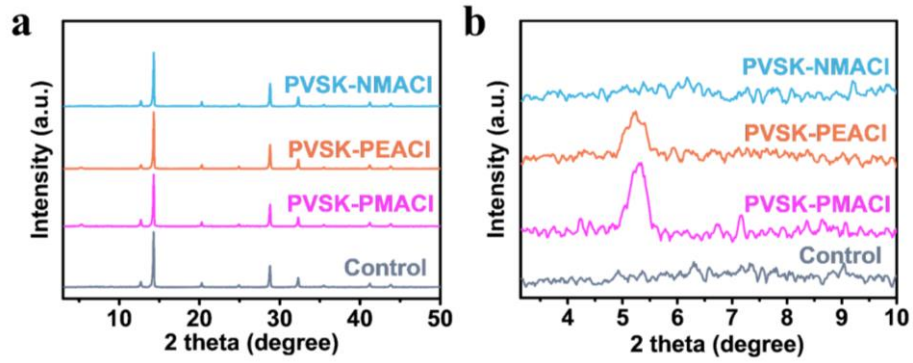
**Fig. S1** Statistical distribution of photovoltaic metrics of PSCs passivated with different PMACl concentrations. **a**  $J_{sc}$ , **b**  $V_{oc}$ , **c** FF, and **d** PCE



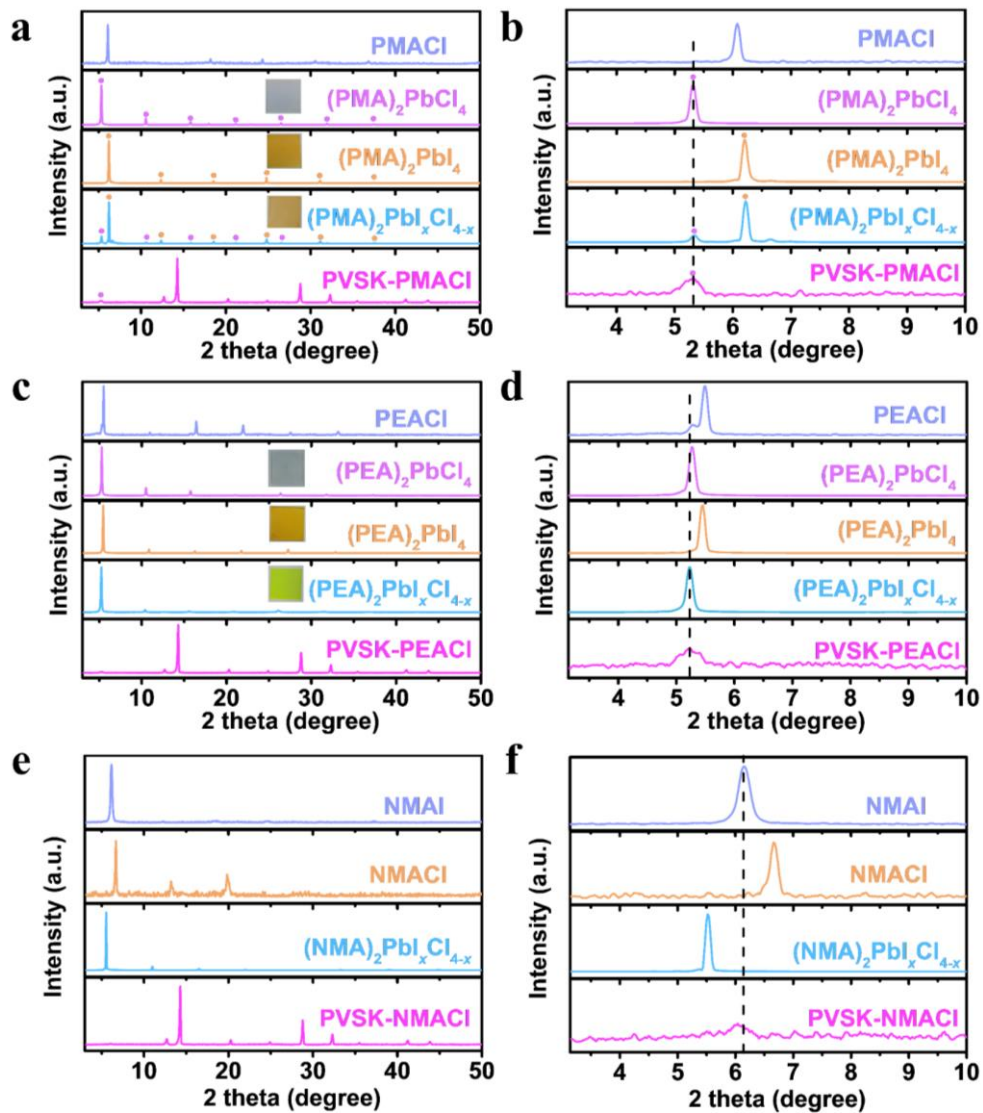
**Fig. S2** Statistical distribution of photovoltaic metrics of PSCs passivated with different PEACl concentration. **a**  $J_{sc}$ , **b**  $V_{oc}$ , **c** FF, and **d** PCE



**Fig. S3** Statistical distribution of photovoltaic metrics of PSCs passivated with different NMACl concentration. **a**  $J_{sc}$ , **b**  $V_{oc}$ , **c** FF, and **d** PCE



**Fig. S4 a** XRD patterns of the control, PVSK-PMACl (3 mg mL<sup>-1</sup>), PVSK-PEACl (2 mg mL<sup>-1</sup>), and PVSK-NMACl (1 mg mL<sup>-1</sup>) films. **b** Enlarged XRD patterns of **a** in the low diffraction angle region



**Fig. S5 a, b** XRD patterns of PVSK-PMACl (3 mg mL<sup>-1</sup>), (PMA)<sub>2</sub>PbCl<sub>4-x</sub>, PMA<sub>2</sub>PbI<sub>4</sub>, (PMA)<sub>2</sub>PbCl<sub>4</sub>, and PMACl. Insets: Photographs of the corresponding films. **c, d** XRD patterns of PVSK-PEACl (2 mg mL<sup>-1</sup>), (PEA)<sub>2</sub>PbCl<sub>4-x</sub>, (PEA)<sub>2</sub>PbI<sub>4</sub>, (PEA)<sub>2</sub>PbCl<sub>4</sub>, and PEACl. Insets: Photographs of the corresponding films. **e, f** XRD patterns of PVSK-NMACl (3 mg mL<sup>-1</sup>), (NMA)<sub>2</sub>PbCl<sub>4-x</sub>, NMACl, and NMAI

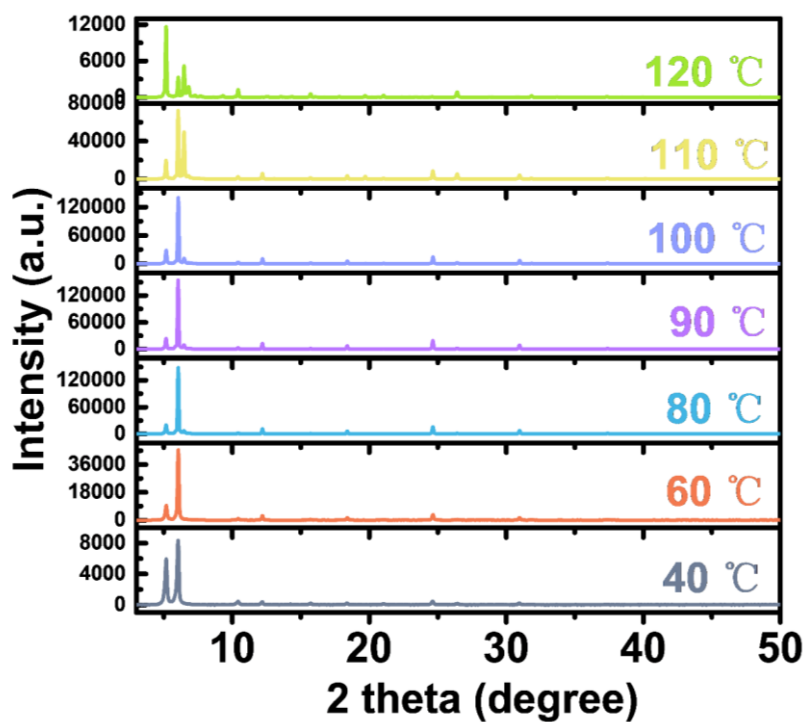


Fig. S6 XRD patterns of 2D (PMA)<sub>2</sub>PbI<sub>x</sub>Cl<sub>4-x</sub> at different annealing temperatures

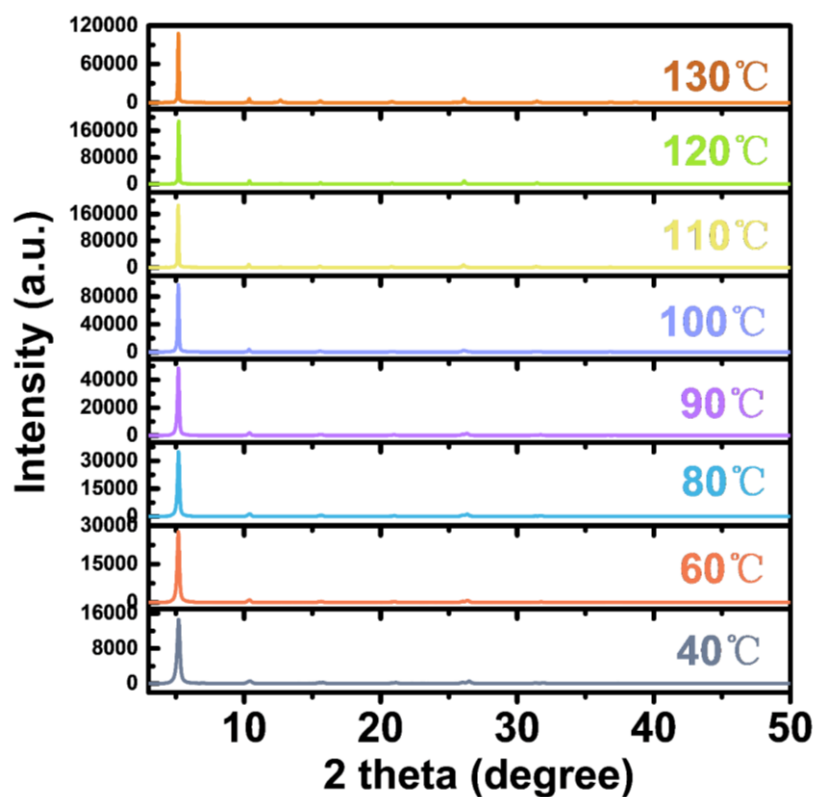
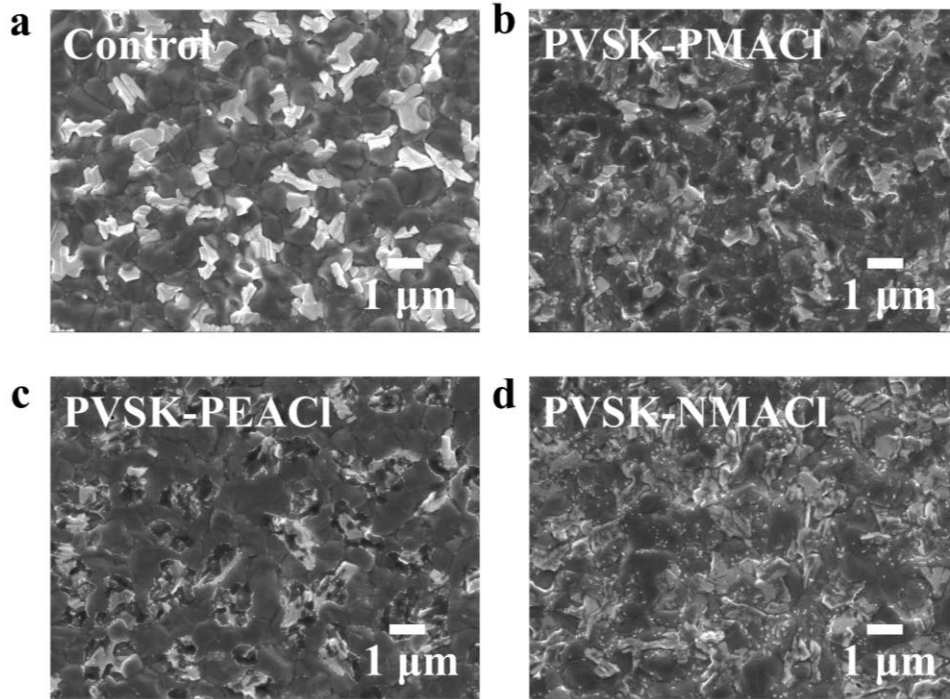
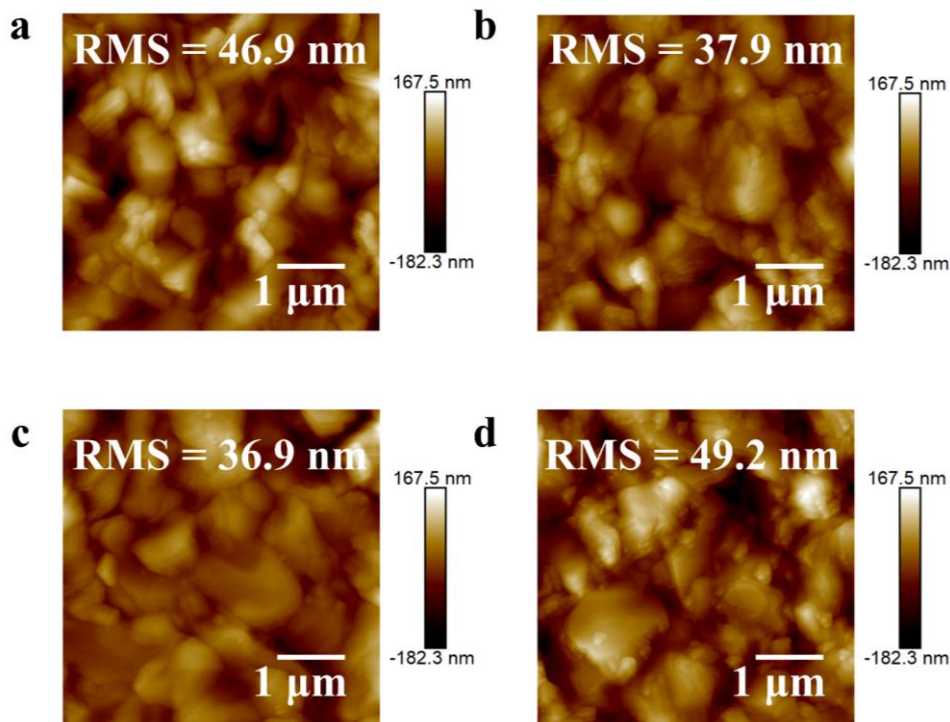


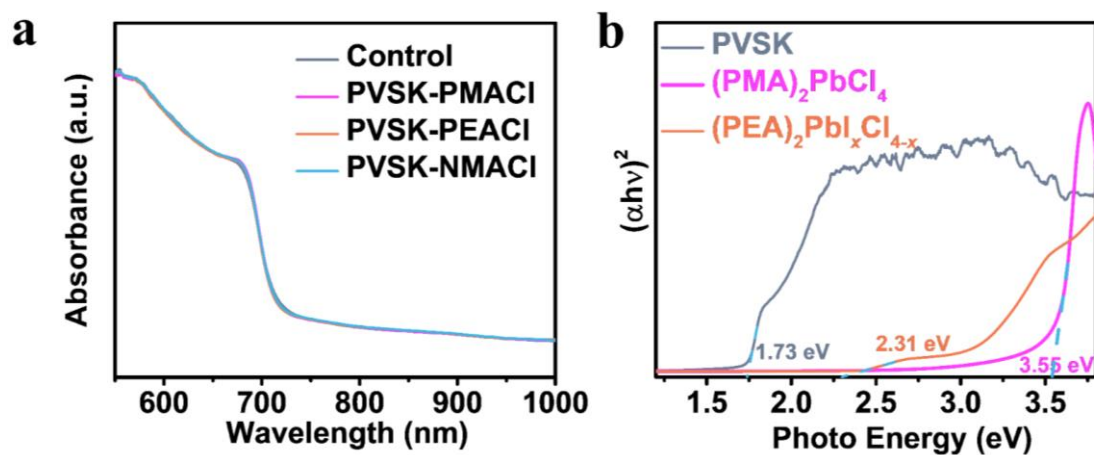
Fig. S7 XRD patterns of 2D (PEA)<sub>2</sub>PbI<sub>x</sub>Cl<sub>4-x</sub> at different annealing temperatures



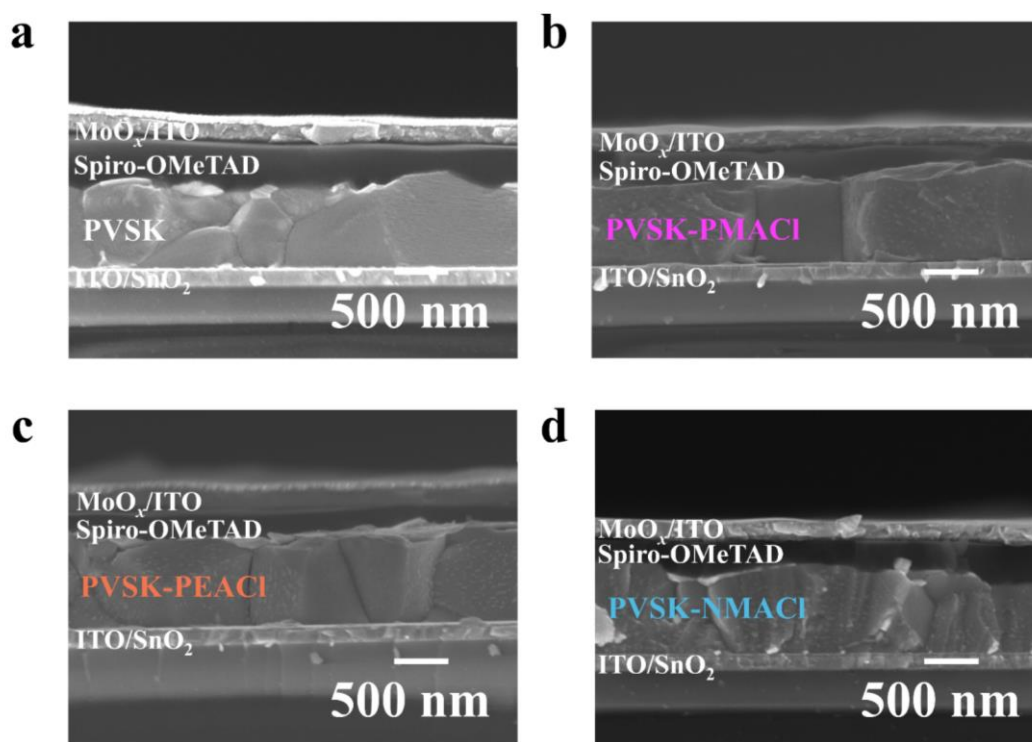
**Fig. S8** Scanning electron microscopy (SEM) images of the **a** control, **b** PVSK-PMACl, **c** PVSK-PEACl, and **d** PVSK-NMACl films



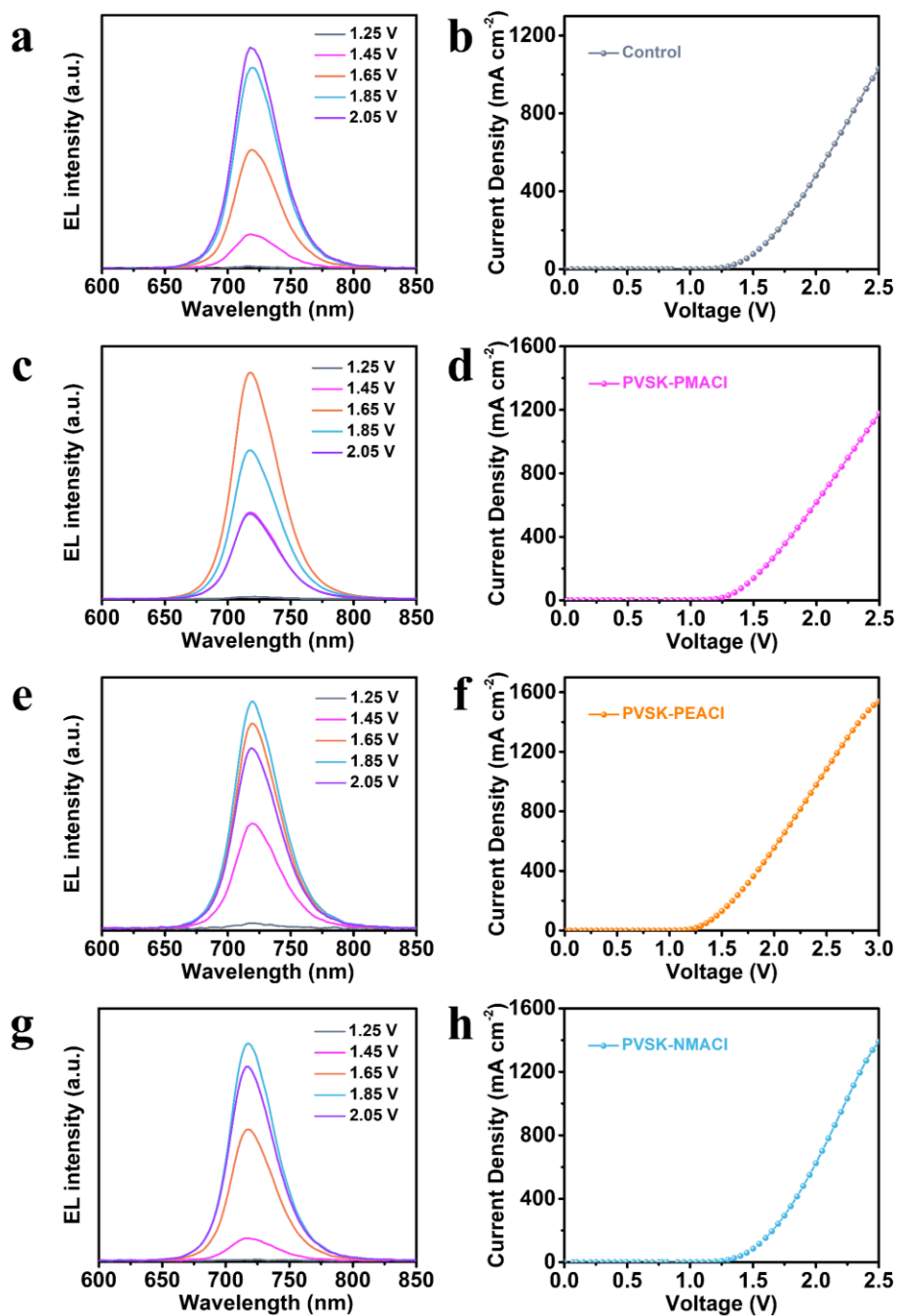
**Fig. S9** Atomic force microscopy (AFM) images of the **a** control, **b** PVSK-PMACl, **c** PVSK-PEACl, and **d** PVSK-NMACl films



**Fig. S10** **a** UV-vis absorption spectra of the control, PVSK-PMACI, PVSK-PEACI, and PVSK-NMACI films. **b** Tauc plot of the control, 2D  $(\text{PMA})_2\text{PbCl}_4$ , and 2D  $(\text{PEA})_2\text{PbI}_x\text{Cl}_{4-x}$  films



**Fig. S11** Cross-sectional SEM images of the device based on the **a** control, **b** PVSK-PMACI, **c** PVSK-PEACI, and **d** PVSK-NMACI films



**Fig. S12** a, c, e, and g EL spectra of the devices based on the control, PVSK-PMACl, PVSK-PEACl, and PVSK-NMACl films operating as LEDs. b, d, f, and h *J-V* curves of the devices based on the control, PVSK-PMACl, PVSK-PEACl, and PVSK-NMACl films

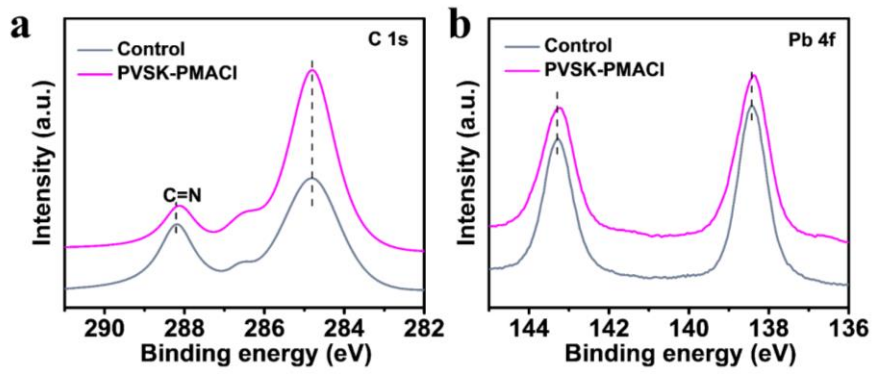


Fig. S13 a C 1s and b Pb 4f XPS spectra of the control and PVSK-PMACl

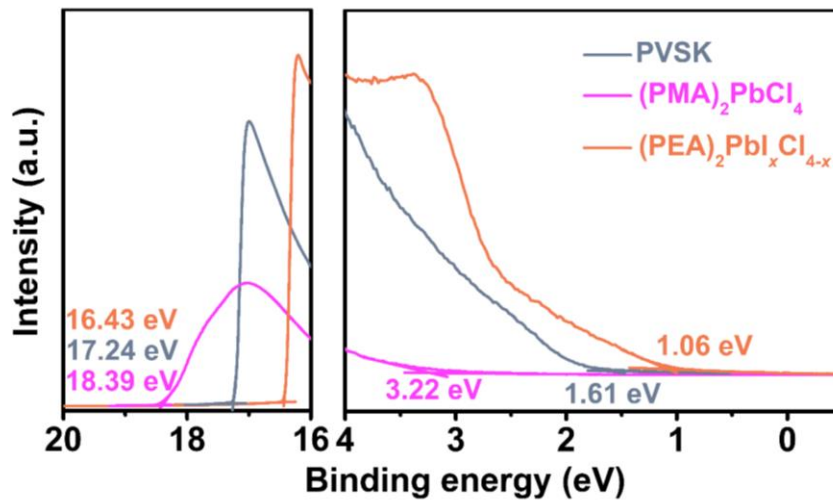


Fig. S14 UPS spectra of the control film, 2D (PMA)<sub>2</sub>PbCl<sub>4</sub>, and 2D (PEA)<sub>2</sub>PbI<sub>x</sub>Cl<sub>4-x</sub>

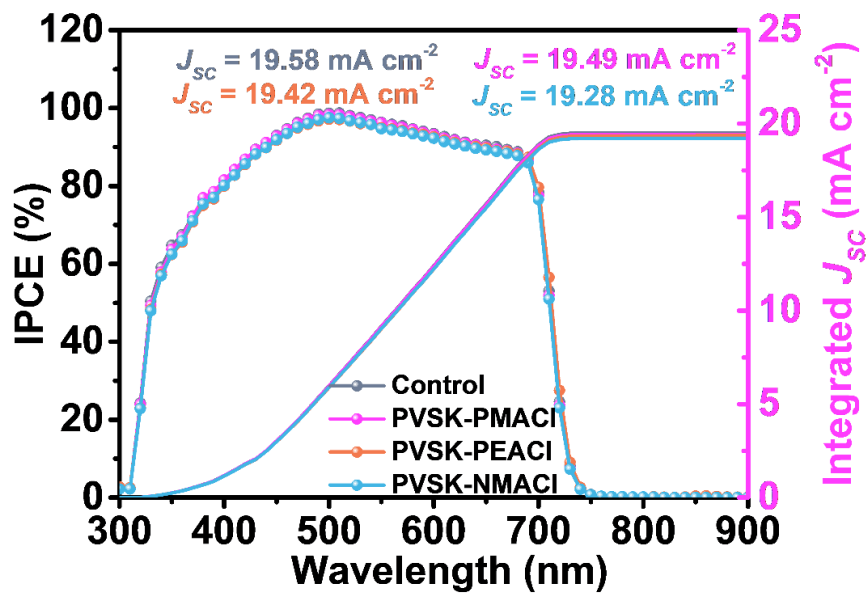


Fig. S15 IPCE and the integrated  $J_{sc}$  for the WBG-PSCs based on the control, PVSK-PMACl, PVSK-PEACl, and PVSK-NMACl films



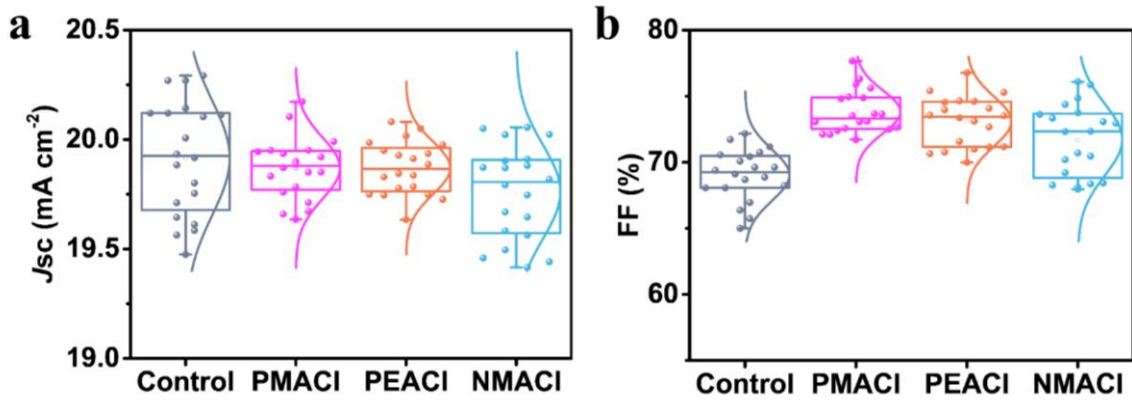


Fig. S16 Statistical results of **a**  $J_{sc}$  and **b** FF of 20 PSCs for each group

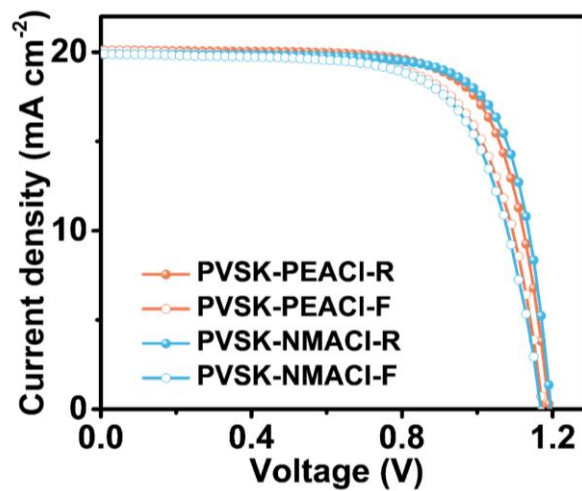


Fig. S17  $J$ - $V$  curves of the WBG-PSCs based on the PVSK-PEACI, and PVSK-NMACI films measured by forward and reverse scans

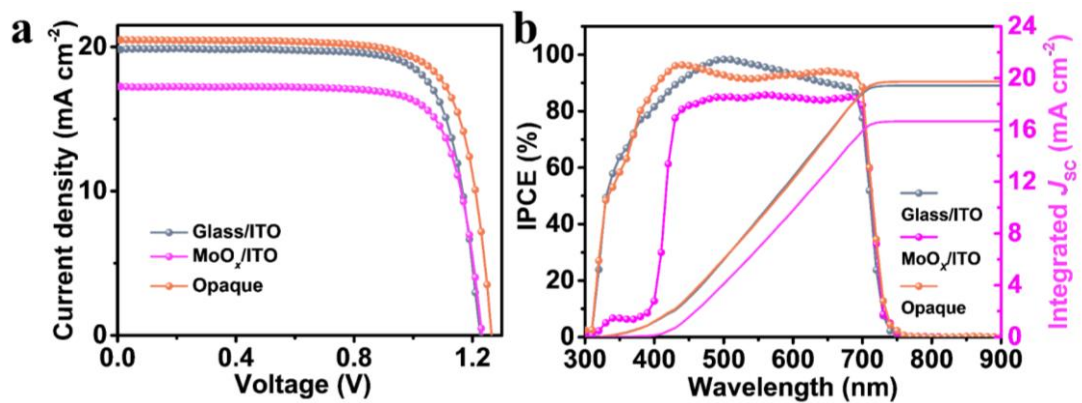
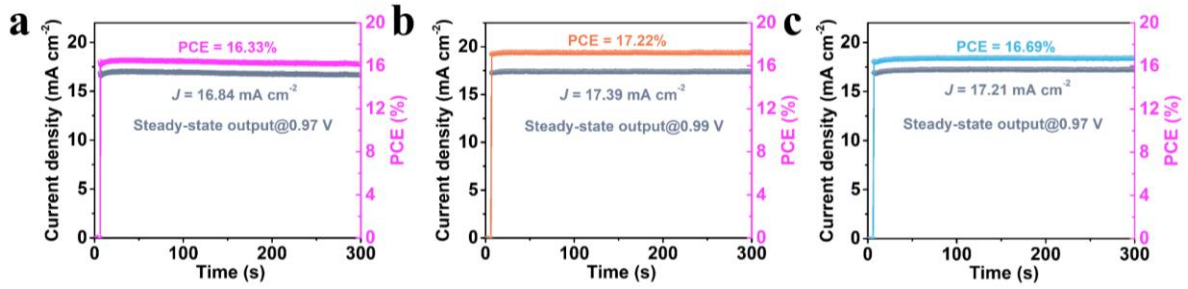
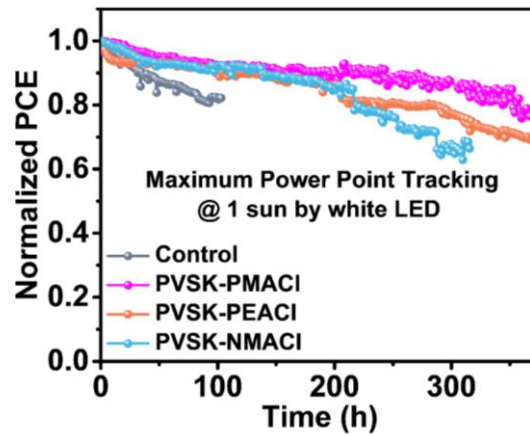


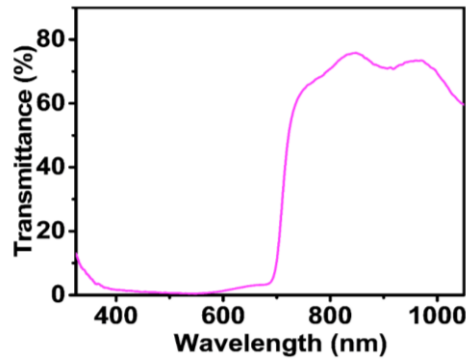
Fig. S18 **a**  $J$ - $V$  curves and **b** IPCE spectra of solar cells. Glass/ITO represents light incident from the glass/ITO side of the semi-transparent cell, MoO<sub>x</sub>/ITO represents light incident from the MoO<sub>x</sub>/ITO side of the semi-transparent cell, and opaque represents the device using Ag electrode



**Fig. S19** Maximum power point tracking of the WBG-PSCs based on the **a** control, **b** PVSK-PEACl, and **c** PVSK-NMAcI films, respectively



**Fig. S20** Maximum power point tracking under white LED lamp with the light intensity of  $100 \text{ mW cm}^{-2}$



**Fig. S21** Transmittance spectrum of semi-transparent WBG-PSCs

**Table S1** XRD peak intensity of 2D  $(\text{PMA})_2\text{PbI}_x\text{Cl}_{4-x}$  annealed at different temperatures

T/°C	40	60	80	90	100	110	120
5.32	5933	9481	20066	23878	28353	19650	11635
6.20	8367	45474	148273	154726	139958	72485	3311
5.32/6.20	0.71	0.21	0.14	0.15	0.20	0.27	3.5

**Table S2** Assignment of the XRD peaks of different 2D perovskites

	(001)	(002)	(003)	(004)	(005)	(006)
(PMA) <sub>2</sub> PbI <sub>4</sub>	6.20	12.34	18.54	24.80	31.12	37.54
(PMA) <sub>2</sub> PbCl <sub>4</sub>	5.32	10.56	15.84	21.14	26.52	31.94
(PMA) <sub>2</sub> Pb(I <sub>1-x</sub> Cl <sub>x</sub> ) <sub>4</sub>	5.32/ 6.20	10.56/ 12.34	15.84 /18.54	21.14/ 24.80	26.52/ 31.12	31.94/ 37.54
(PEA) <sub>2</sub> PbI <sub>4</sub>	5.46	10.84	16.28	21.74	27.26	32.86
(PEA) <sub>2</sub> PbCl <sub>4</sub>	5.28	10.50	15.74	21.04	26.38	31.76
(PEA) <sub>2</sub> Pb(I <sub>1-x</sub> Cl <sub>x</sub> ) <sub>4</sub>	5.22	10.40	15.58	20.80	26.06	31.40

**Table S3** Fitted parameters of TRPL results of the control, PVSK-PMACl, PVSK-PEACl, and PVSK-NMACl films

Samples	$\tau_1$ /ns	A <sub>1</sub>	$\tau_2$ /ns	A <sub>2</sub>	$\tau_{avg}$ (ns)
Control	79.3	0.7	353.2	0.8	309.5
PVSK-PMACl	167.6	0.3	962.9	0.8	914.1
PVSK-PEACl	111.4	0.9	816.6	0.5	675.9
PVSK-NMACl	98.1	1.1	474.4	0.6	369.4

**Table S4** Photovoltaic parameters of the devices based on the control, PVSK-PMACl, PVSK-PEACl, and PVSK-NMACl films measured by forward and reverse scans

Samples	Scanning direction	$J_{SC}$ (mA cm <sup>-2</sup> )	$V_{oc}$ (V)	FF (%)	PCE (%)	HI (%)
Control	Reverse	19.71	1.181	70.98	16.52	15.25
	Forward	19.70	1.163	61.09	14.00	
PVSK-PMACl	Reverse	19.78	1.224	75.91	18.38	4.19
	Forward	19.75	1.207	73.82	17.62	
PVSK-PEACl	Reverse	20.10	1.191	73.13	17.51	6.85
	Forward	20.09	1.174	69.17	16.31	
PVSK-NMACl	Reverse	19.91	1.196	74.86	17.82	9.99
	Forward	19.91	1.169	68.92	16.04	

**Table S5** Champion photovoltaic parameters of solar cells. Glass/ITO represents light incident from the glass/ITO side of the semi-transparent cell, MoO<sub>x</sub>/ITO represents light incident from the MoO<sub>x</sub>/ITO side of the semi-transparent cell, and opaque represents the device using Ag electrode

Samples	$J_{SC}$ (mA cm <sup>-2</sup> )	$V_{OC}$ (V)	FF (%)	PCE (%)
Glass/ITO	19.87	1.23	76.31	18.60
MoO <sub>x</sub> /ITO	17.26	1.23	77.19	16.42
Opaque	20.49	1.27	75.68	19.62