Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Interfacial Engineering of ZnO Electron Transporting Layer by Self-Assembled Monolayers for High Performance and Stable Perovskite Solar Cells

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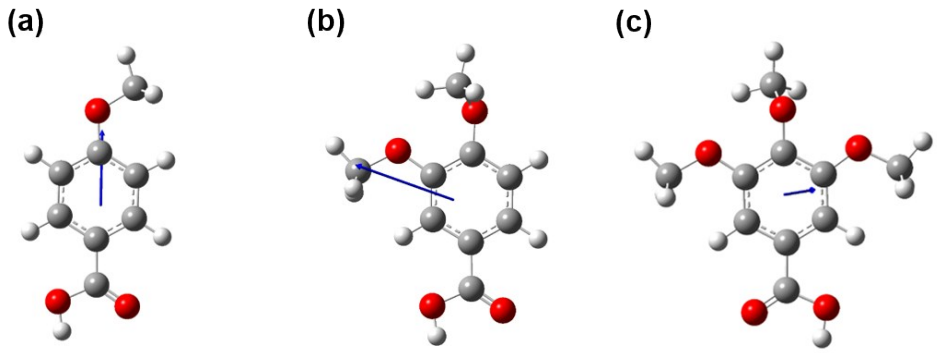

Figure S1. Chemical structures of (a) MBA, (b) DMBA and (c) TMBA respectively.

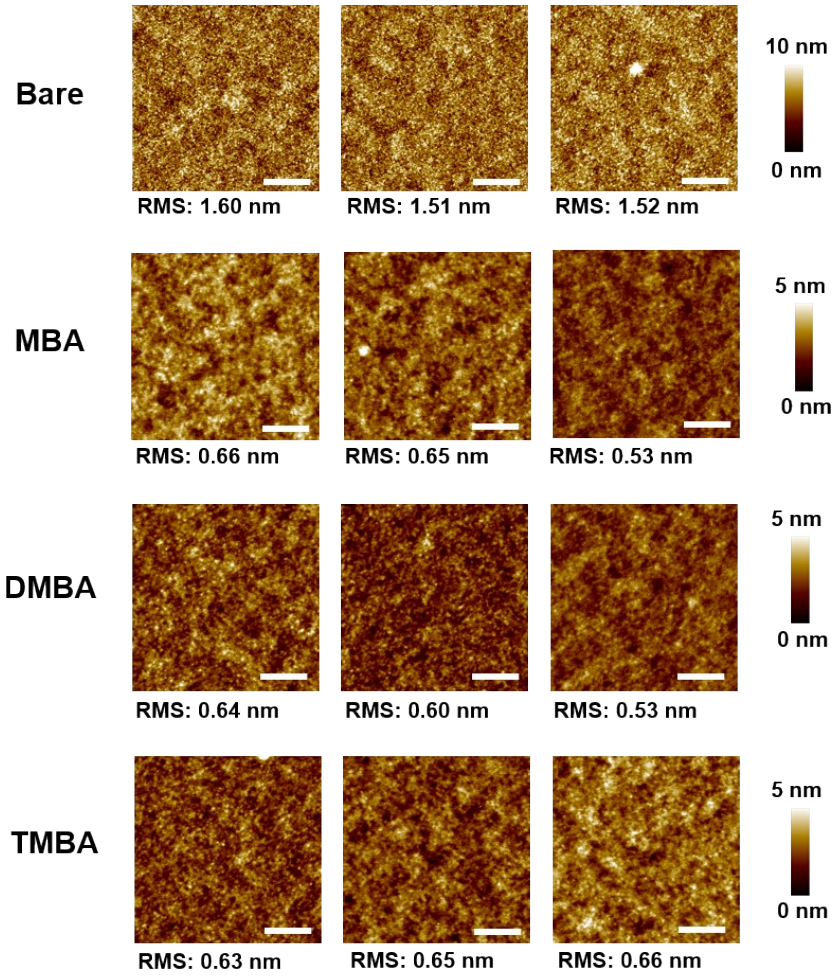

Figure S2. AFM topography images of ZnO with and without SAM treatment. All the scale bars are 0.5 μm.

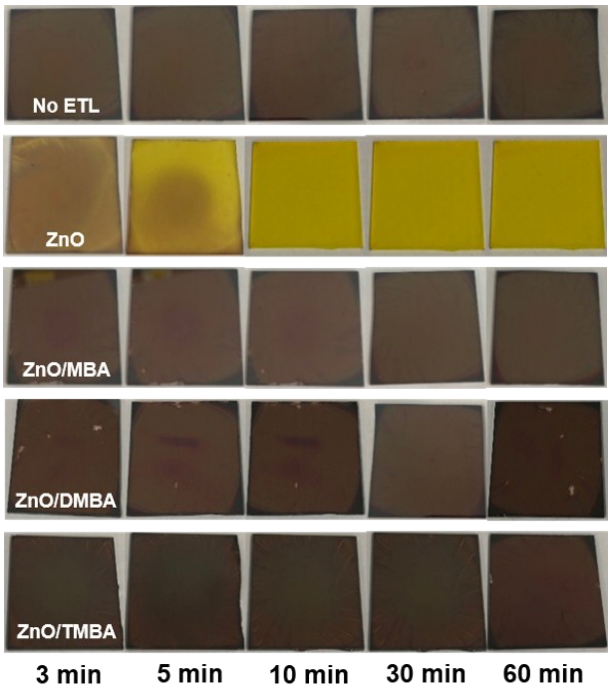

Figure S3. Photographs of perovskite films on ZnO ETLs heated at 100 °C for the designated time.

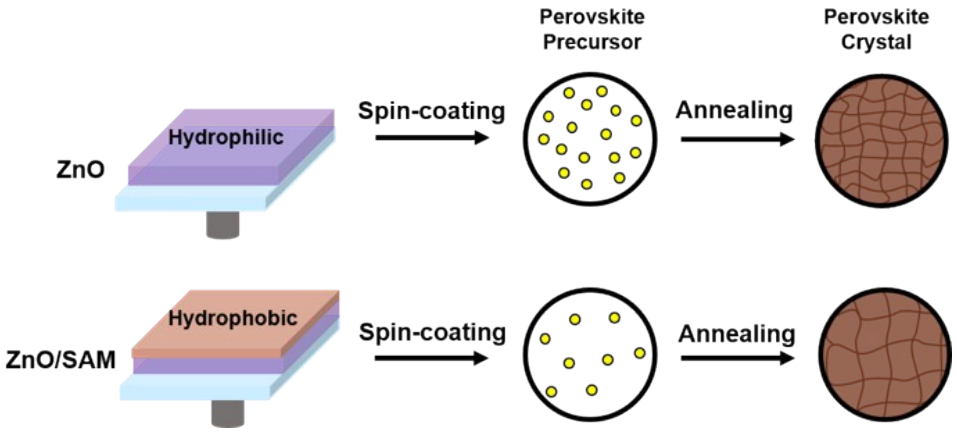

Figure S4. Illustration for the mechanism of enhancing perovskite nucleation time.

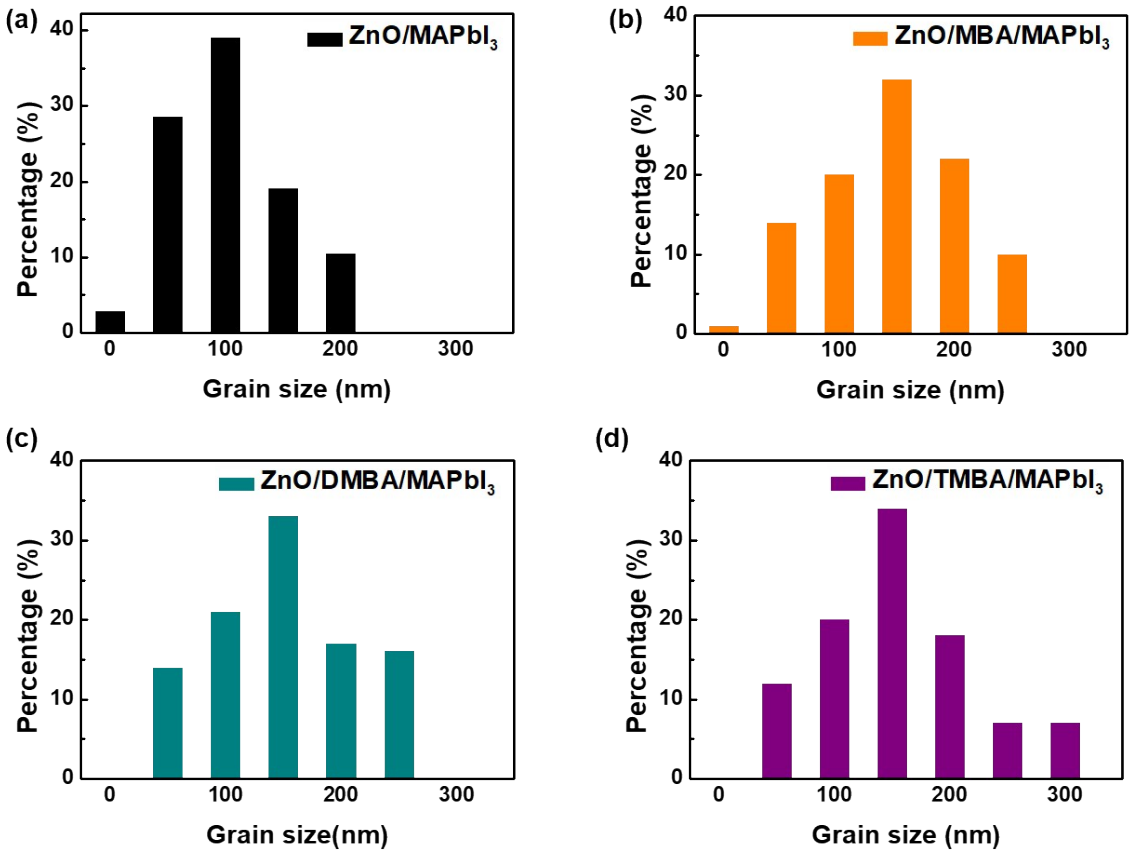

Figure S5. Statistic distributions of perovskite grain sizes extracted from SEM images for (a) $ZnO/CH_3NH_3PbI_3$, (b) $ZnO/MBA/CH_3NH_3PbI_3$, (c) $ZnO/DMBA/CH_3NH_3PbI_3$, and (d) $ZnO/TMBA/CH_3NH_3PbI_3$.

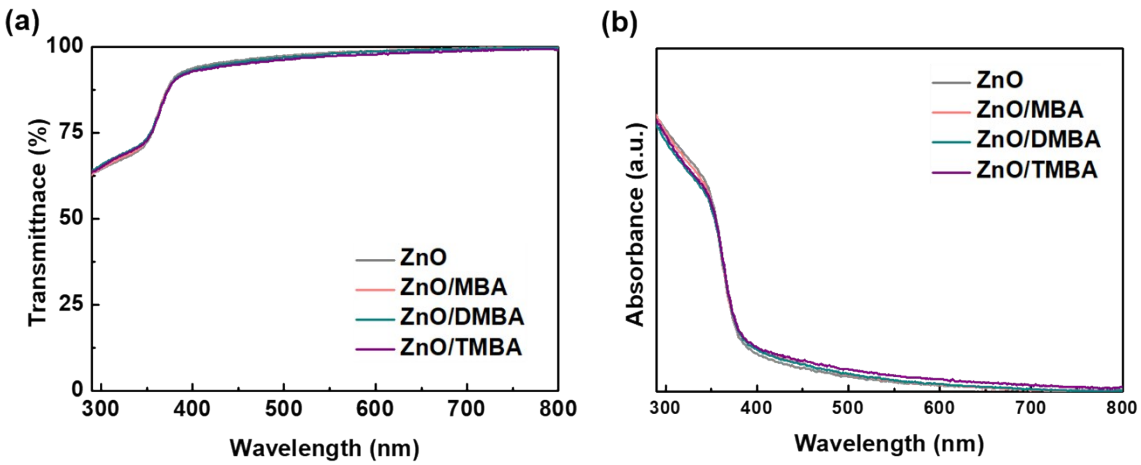

Figure S6. (a) Transmittance spectra of the ZnO ETLs with and without SAM treatment. (b) UV-vis absorption spectra of ZnO ETLs with and without SAM treatment.

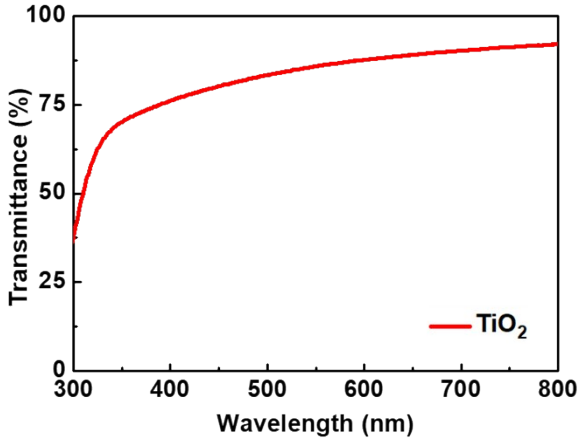

Figure S7. Transmittance spectrum of the conventional TiO_2 ETLs.

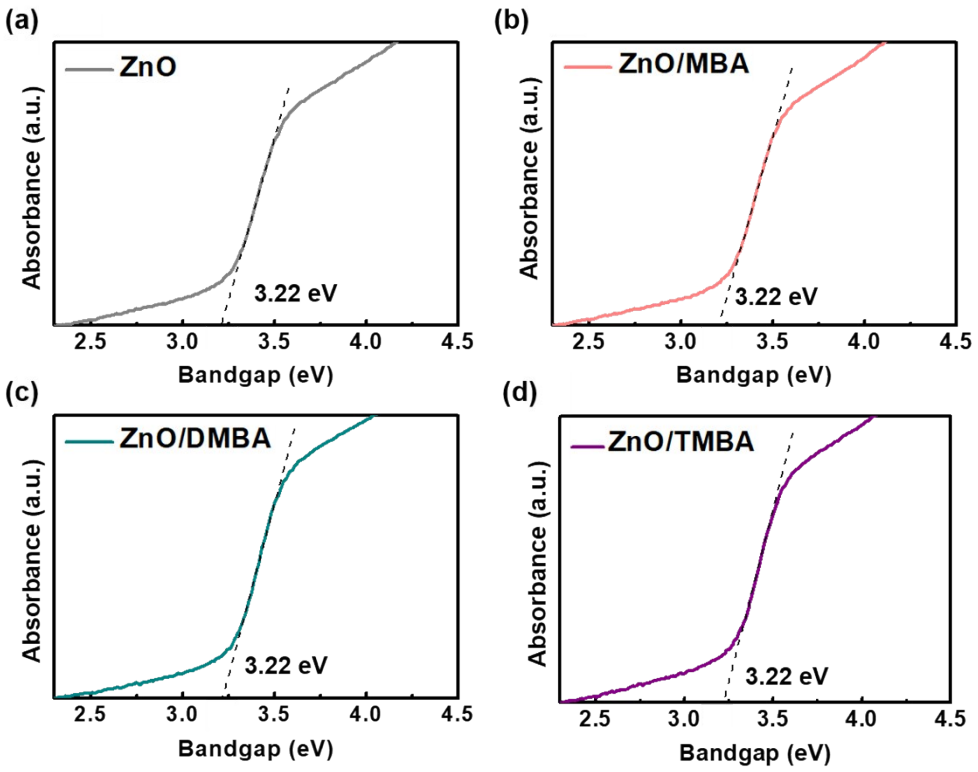

Figure S8. Optical bandgaps of (a) ZnO (b) ZnO/MBA (c) ZnO/DMBA, and (d) ZnO/TMBA.

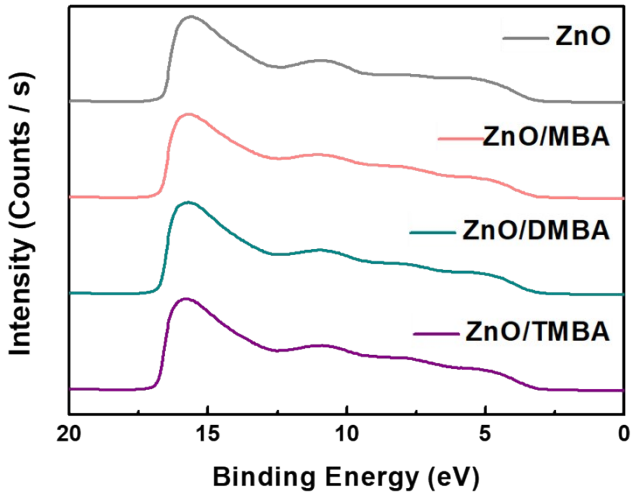

Figure S9. UPS spectra of ZnO ETLs with and without SAM treatment.

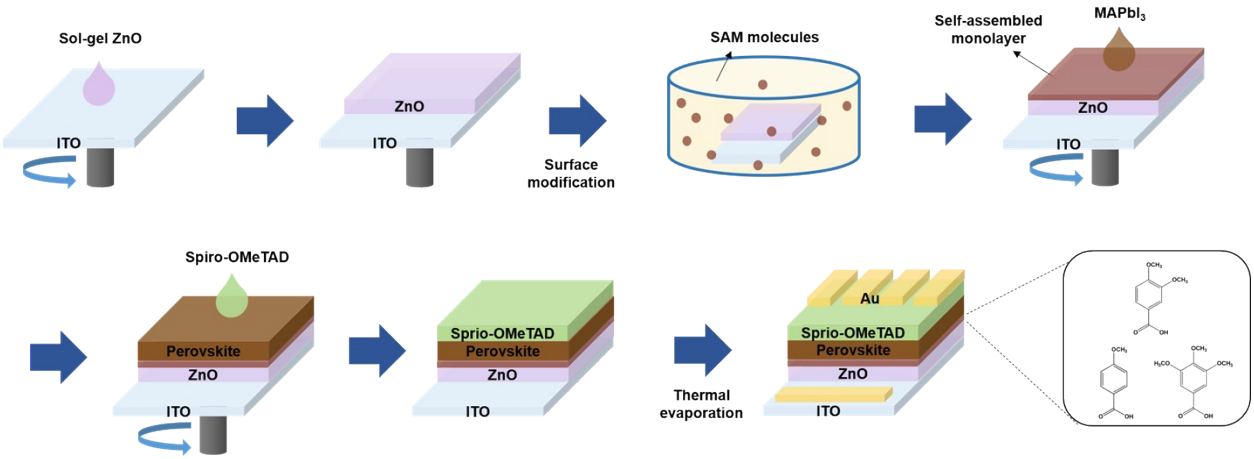

Figure S10. Illustration for perovskite solar cell fabrication

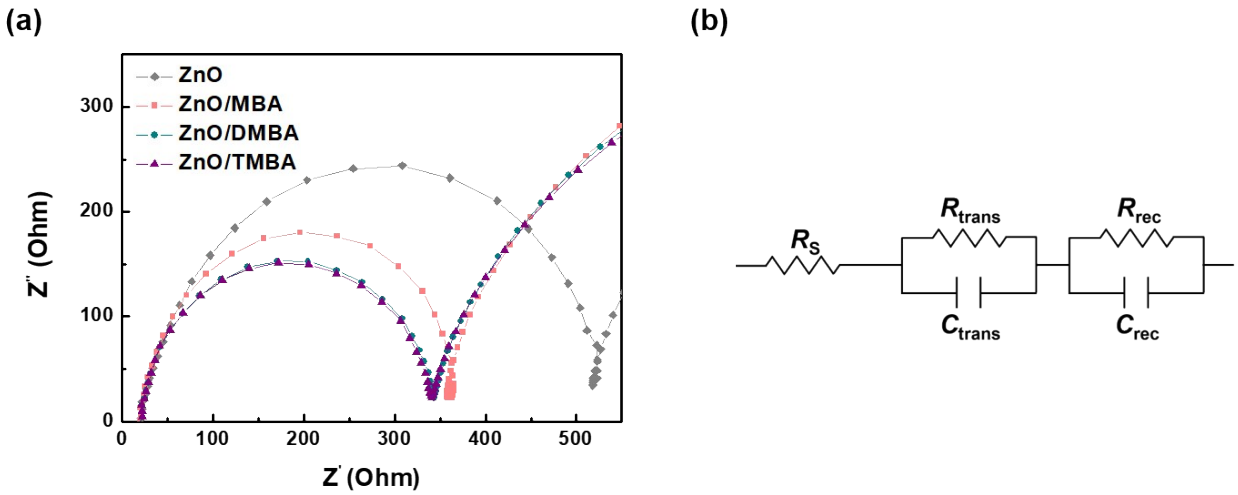

Figure S11. (a) Nyquist plots of perovskite solar cells with and without interfacial engineering with SAMs, (b) Equivalent circuit model used to fit the Nyquist plots.

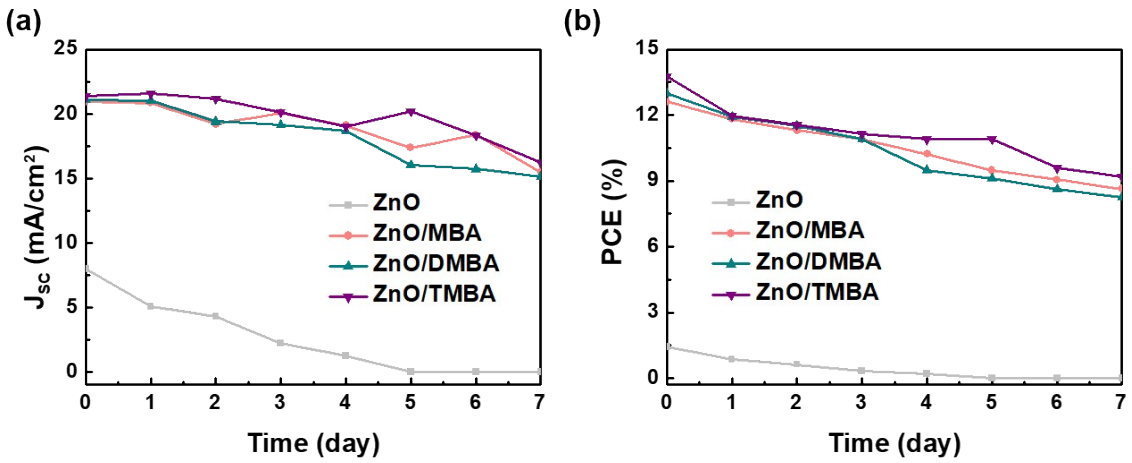

Figure S12. Photovoltaic performance decay curves of PSCs stored in ambient air with RH of 45% at 28 °C (a) PCE, (b) J_{SC}.

Table S1. DFT calculating results of MA-SAMs

Sample	x	y	z	Total
MA-MBA	-8.5456	-6.2564	0.9119	10.6302
MA-DMBA	12.4074	4.1771	3.5350	13.5606
MA-TMBA	-12.6416	-2.6662	3.1496	13.2981

Table S2. The initial absolute photovoltaic parameters for 18 perovskite solar cells. The device configuration is ITO/ZnO/$MAPbI_3$/Spiro-OMeTAD/Au. The best performance of the device is denoted as red.

V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
0.82	7.97	21.98	1.44
1.03	5.30	15.76	0.86
0.24	11.55	24.41	0.67
0.94	10.17	12.92	1.24
0.83	5.12	20.87	0.86
0.87	6.25	18.16	0.98
0.88	6.23	18.49	1.01
0.92	5.85	20.51	1.11
0.52	8.24	22.96	0.99
0.89	5.91	18.81	0.98
0.74	6.18	19.29	0.88
0.82	3.63	19.81	0.60
0.83	7.10	20.35	1.19
0.88	4.99	19.23	0.85
0.88	4.77	13.06	0.55
1.05	5.79	13.66	0.83
1.08	7.03	14.67	1.08
1.03	5.08	16.43	0.86

Table S3. The initial absolute photovoltaic parameters for 18 perovskite solar cells. The device configuration is ITO / ZnO / MBA / $MAPbI_3$ / Spiro-OMeTAD / Au. The best performance of the device is denoted as red.

V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
0.98	20.95	61.18	12.60
1.02	20.39	54.99	11.49
1.00	21.29	53.56	11.35
0.99	20.43	60.84	12.25
1.03	21.00	49.24	10.68
1.00	19.39	62.10	12.03
0.98	19.02	61.36	11.44
1.00	19.69	62.09	12.17
1.03	20.00	60.84	12.54
1.01	20.46	55.79	11.51
1.03	20.38	58.25	12.25
0.99	20.14	57.99	11.53
0.99	21.61	55.36	11.86
0.99	19.22	56.40	10.77
0.96	21.64	56.88	11.79
0.96	21.61	56.00	11.62
1.03	19.52	57.35	11.52
1.02	19.48	57.35	11.35

Table S4. The initial absolute photovoltaic parameters for 18 perovskite solar cells. The device configuration is ITO / ZnO / DMBA / $MAPbI_3$ / Spiro-OMeTAD / Au. The best performance of the device is denoted as red.

V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
1.03	21.40	58.37	12.86
0.95	21.08	58.41	11.64
1.01	21.30	54.48	11.69
1.03	20.94	49.78	10.77
1.00	21.11	59.89	12.66
1.04	20.03	55.66	11.58
1.03	21.01	56.38	12.25
0.99	20.34	63.59	12.86
1.02	20.86	57.67	12.24
1.01	19.57	60.77	11.98
1.01	22.20	55.81	12.67
1.00	19.92	61.76	12.34
1.01	21.13	60.54	12.97
1.01	20.39	61.77	12.79
0.99	21.72	60.06	12.90
1.02	21.09	56.22	12.10
1.00	22.33	52.45	11.66
0.98	19.52	56.39	10.75

Table S5. The initial absolute photovoltaic parameters for 18 perovskite solar cells. The device configuration is ITO / ZnO / TMBA / $MAPbI_3$ / Spiro-OMeTAD / Au. The best performance of the device is denoted as red.

V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
1.01	22.85	53.29	12.24
1.02	21.87	56.03	12.44
1.05	21.38	60.96	13.75
1.03	21.44	59.72	13.17
1.04	21.82	58.73	13.28
1.02	21.45	60.22	13.24
1.05	22.22	54.08	12.49
1.01	22.32	55.35	12.54
1.02	22.17	57.28	13.00
1.01	21.22	58.68	12.45
1.02	22.09	55.88	12.64
1.02	21.70	57.68	12.82
1.00	22.75	55.07	12.50
1.03	22.77	58.40	13.66
1.06	20.97	61.61	13.68
1.03	22.58	57.55	13.36
1.07	22.14	53.05	12.61
1.06	20.49	53.78	11.65