

Supporting Information

An effective surface modification strategy with high reproducibility for simultaneously improving efficiency and stability of inverted MA- free perovskite solar cells

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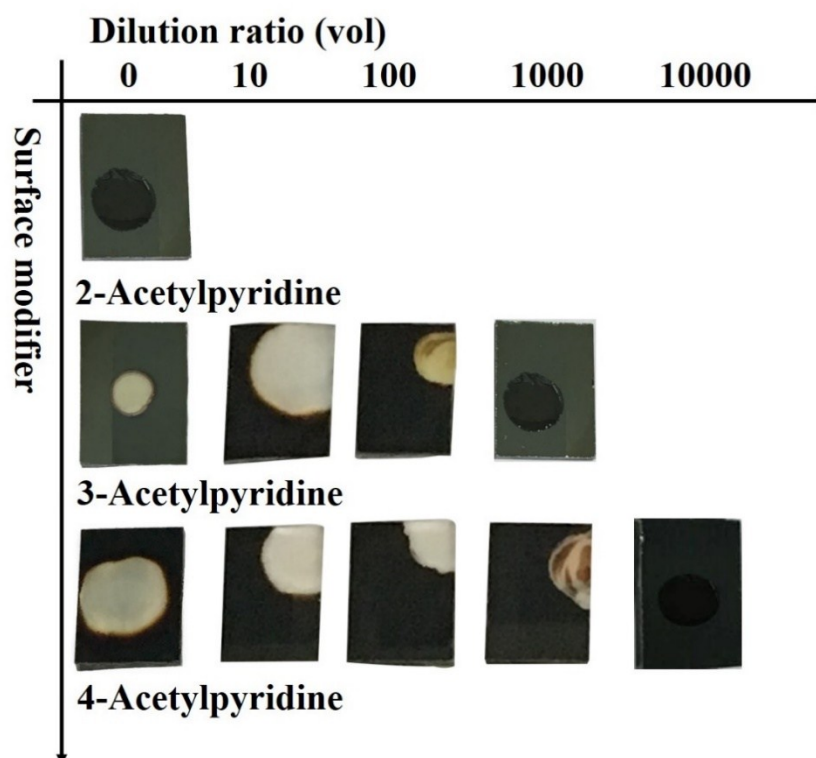


Figure S1. Optical photographs of the corresponding states when one drop of surface modification solution (diluted in diethyl ether with different dilution ratios) was dropped on the surface of perovskite films.

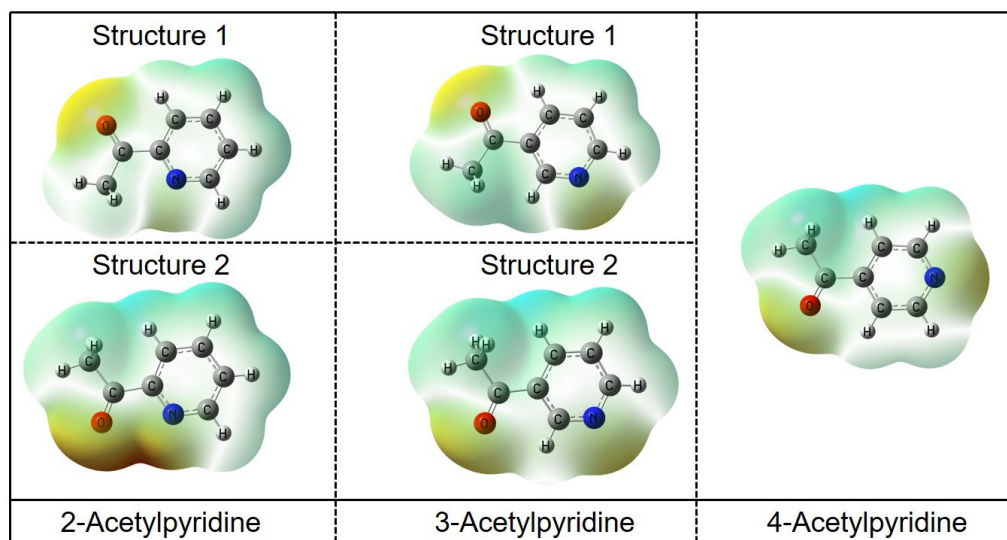


Figure S2. Calculated dipole moments of the surface modifiers used in this work.

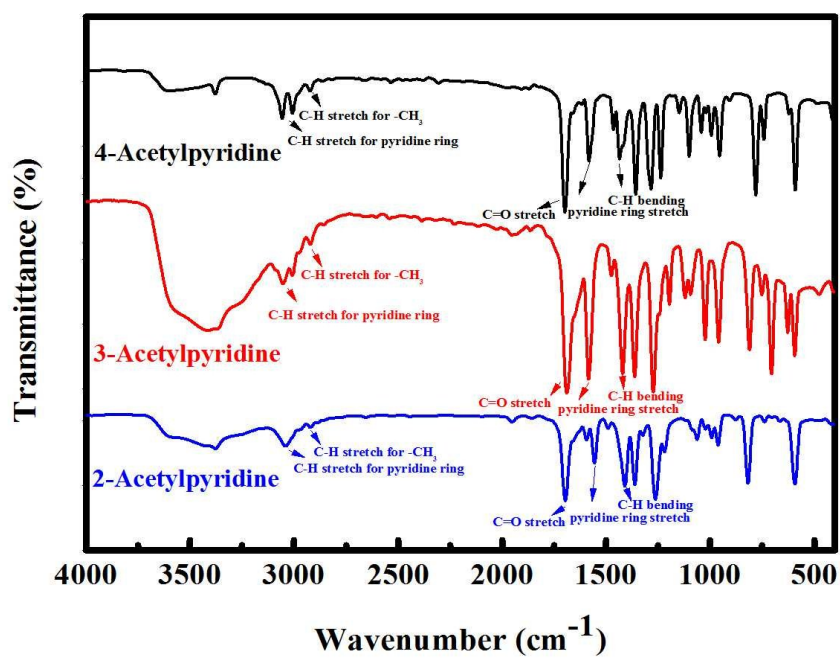


Figure S3. FT-IR spectroscopy of the surface modifiers used in this work (2-Acetylpyridine, 3-Acetylpyridine, and 4-Acetylpyridine).

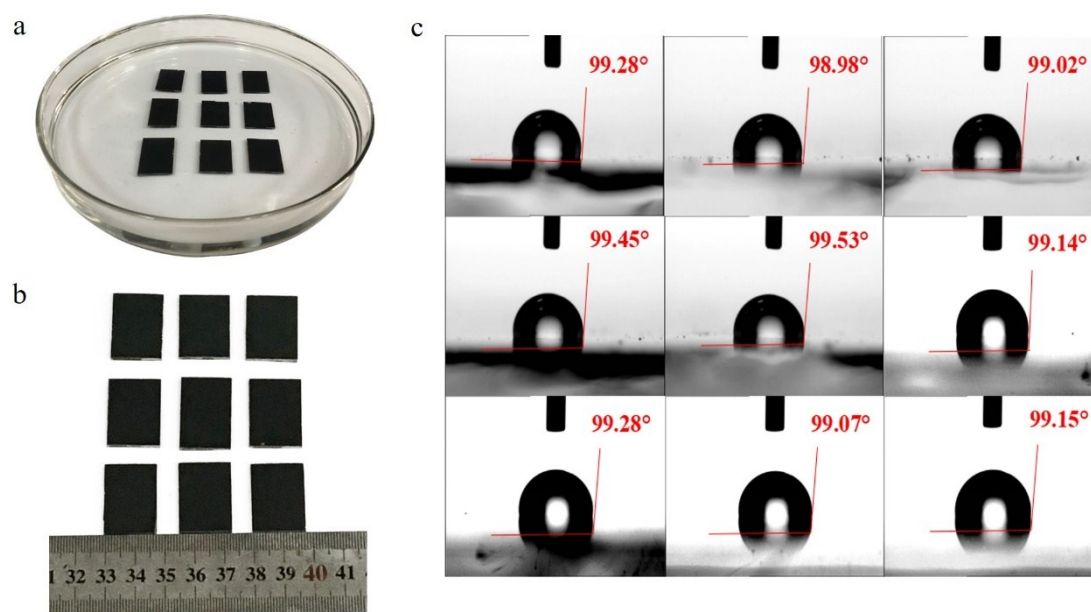


Figure S4. (a) Optical photographs of the process of surface modification. (b) Optical photographs of the perovskite films after surface modification treatment. (c) The corresponding contact angle test results of the modified perovskite films shown in (b).

Supplementary Table S1.

Performance parameters of the PSCs based on the perovskite films treated with different surface modifiers.

Condition	J_{sc} (mA•cm ⁻²)	V_{oc} (V)	FF (%)	PCE (%)	Series resistances (Ω •cm ²)	Shunt resistances (Ω •cm ²)
Pristine	20.73±1.37	0.96±0.07	70.46±3.12	15.68±1.07	5.52±0.31	652.38±326.71
2-Acetylpyridine	22.58±0.65	1.06±0.02	78.51±1.41	19.07±0.98	4.21±0.08	2779.29±153.26
3-Acetylpyridine	21.88±0.92	1.02±0.04	75.19±2.02	17.65 ±1.01	4.73±0.15	2128.85±239.81
4-Acetylpyridine	21.66±0.96	1.00±0.05	74.1±2.39	17.12±1.03	4.86±0.17	1284.3±262.73

Supplementary Table S2. Summary of the photovoltaic parameters for the PSCs with and without surface modification before and after aging (maintained in ambient at room temperature), scanning mode: forward scan (from -0.2 V to 1.2 V).

Devices	Condition @Stored in ambient air	<i>J</i>_{sc} (mA•cm⁻²)	<i>V</i>_{oc} (V)	FF (%)	PCE (%)	PCE /PCE_{initial}
Pristine	Fresh	21.98	1.03	73.41	16.62	100%
	Aged, 2000h	11.07	0.85	54.71	5.15	31%
2-Acetylpyridine	Fresh	23.07	1.08	79.44	19.79	100%
	Aged, 2000h	22.31	1.07	78.75	18.8	95%
3-Acetylpyridine	Fresh	22.74	1.06	77.01	18.56	100%
	Aged, 2000h	21.51	1.04	68.04	15.22	82%
4-Acetylpyridine	Fresh	22.57	1.05	76.46	18.12	100%
	Aged, 2000h	20.86	1.01	64.5	13.59	75%

Supplementary Table S3. Summary of the photovoltaic parameters for the PSCs with and without surface modification before and after aging (thermal aging @ 85°C in the dark in an N₂ atmosphere), scanning mode: forward scan (from -0.2 V to 1.2 V)

Devices	Condition @ thermal aging at 85°C	<i>J</i>_{sc} (mA•cm⁻²)	<i>V</i>_{oc} (V)	FF (%)	PCE (%)	PCE /PCE_{initial}
Pristine	Fresh	21.99	1.03	73.47	16.64	100%
	Aged, 500h	14.67	0.95	65.65	9.15	55%
2-Acetylpyridine	Fresh	23.05	1.08	79.71	19.84	100%
	Aged, 500h	21.73	1.07	77.16	17.94	90.4%
3-Acetylpyridine	Fresh	22.76	1.06	77.01	18.58	100%
	Aged, 500h	20.91	1.03	64.72	13.94	75%
4-Acetylpyridine	Fresh	22.57	1.05	76.33	18.09	100%
	Aged, 500h	20.38	1.01	60.63	12.48	69%

Supplementary Table S4. Summary of the photovoltaic parameters for the PSCs with and without surface modification before and after aging (light soaking @ N₂, near MPP, at 45 °C), scanning mode: forward scan (from -0.2 V to 1.2 V).

Devices	Condition @ light soaking, MPP, 45 °C	<i>J</i>_{sc} (mA•cm⁻²)	<i>V</i>_{oc} (V)	FF (%)	PCE (%)	PCE /PCE_{initial}
Pristine	Fresh	22.03	1.03	73.64	16.71	100%
	Aged, 500h	14.19	0.94	63.05	8.41	50.3%
2-Acetylpyridine	Fresh	23.03	1.08	79.65	19.81	100%
	Aged, 500h	22.17	1.07	76.51	18.15	91.6%
3-Acetylpyridine	Fresh	22.76	1.06	76.89	18.55	100%
	Aged, 500h	20.56	1.04	69.73	14.91	80.4%
4-Acetylpyridine	Fresh	22.57	1.05	76.33	18.09	100%
	Aged, 500h	20.64	1.01	62.03	12.93	71.5%