

Supporting Information

Mechanism of Water Effect on Enhancing the Photovoltaic Performance of Triple-Cation Hybrid Perovskite Solar Cells

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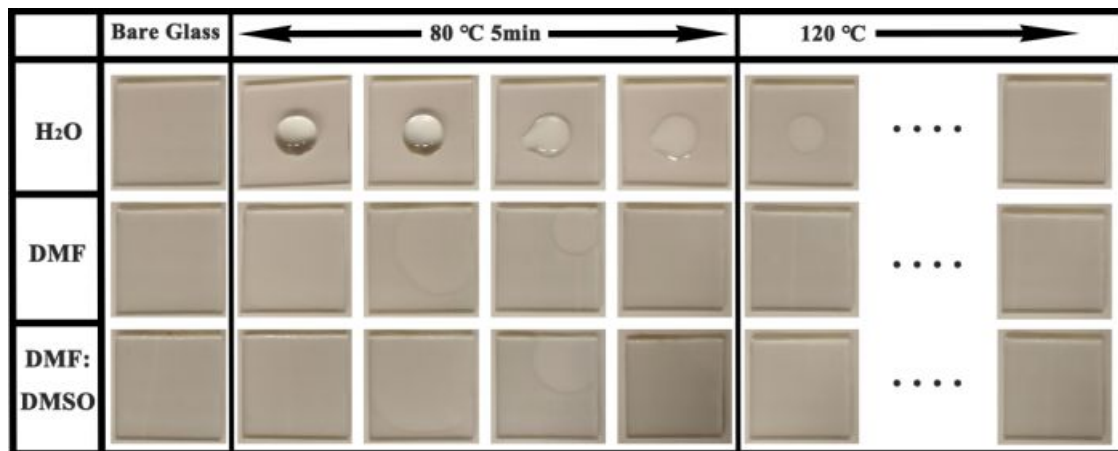


Figure S1. Thermal experiment on H₂O, DMF and DMF:DMSO.

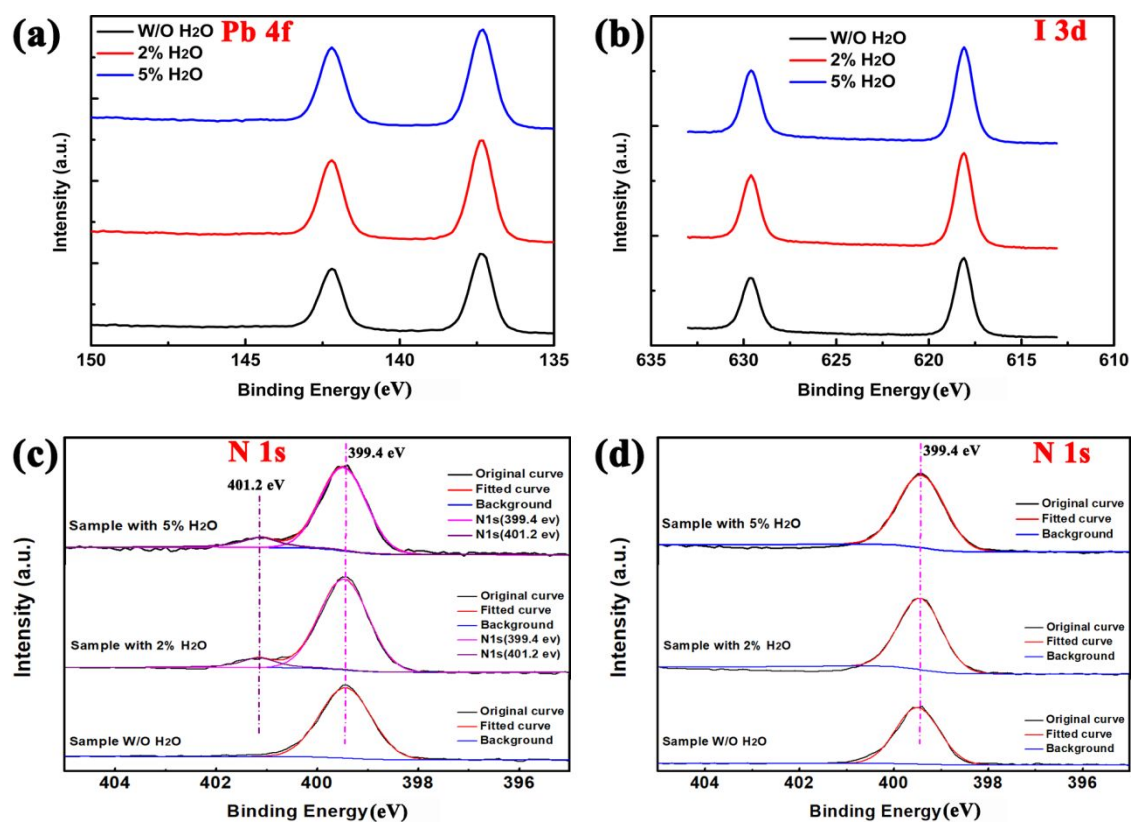


Figure S2. XPS spectra of (a) Pb4f, (b) I3d, (c) N1s for FA films and (d) N1s for 2nd-A films.

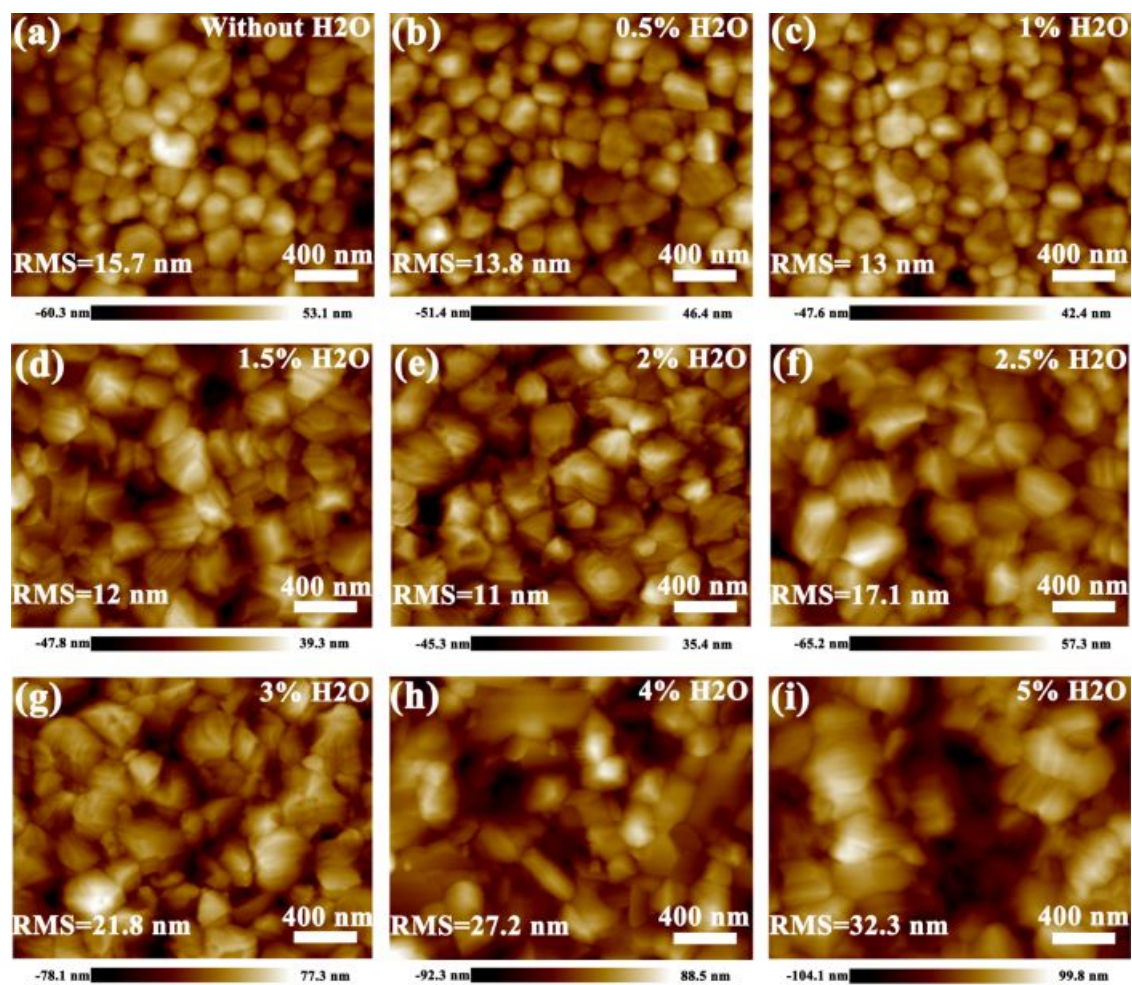


Figure S3. AFM images of 2nd-A films with (a) 0%, (b) 0.5%, (c) 1%, (d) 1.5%, (e) 2%, (f) 2.5%, (g) 3%, (h) 4% and (i) 5% H₂O.

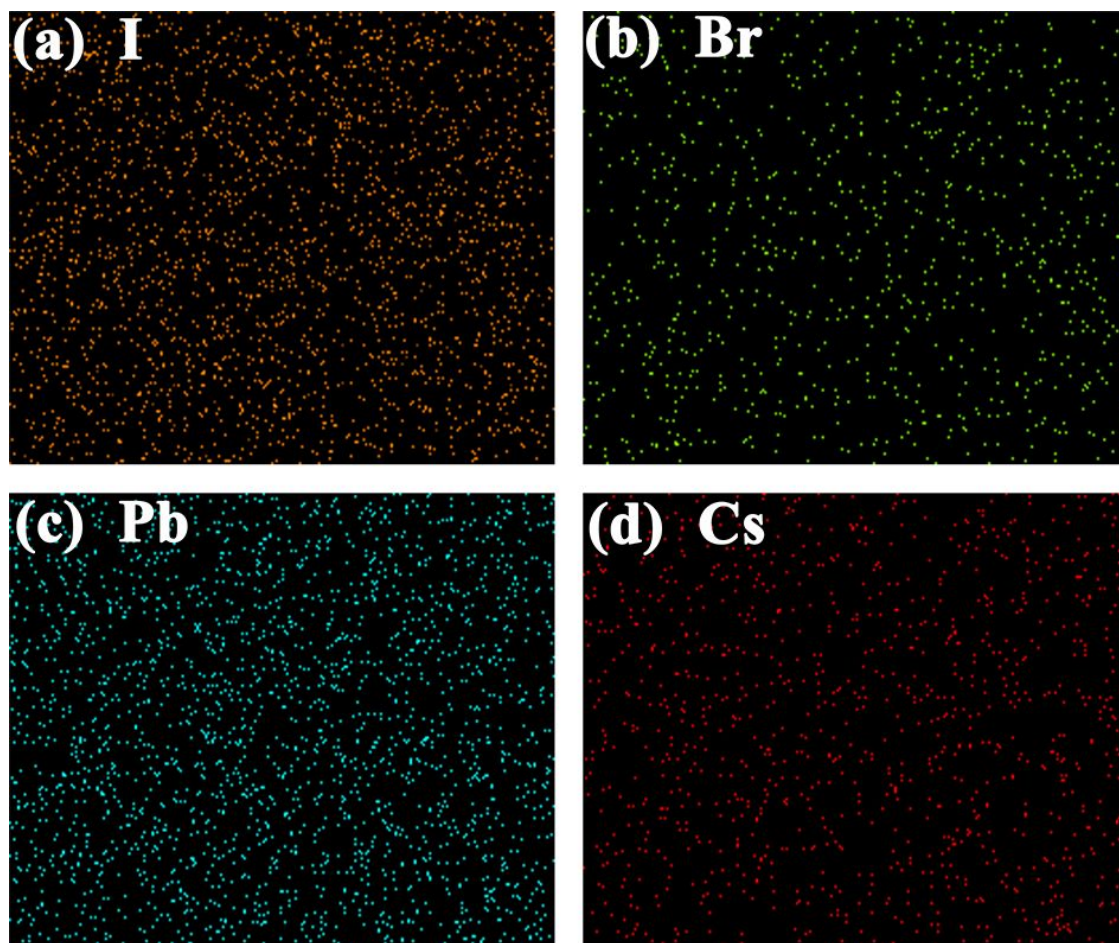


Figure S4. EDX elemental mapping of (a) I, (b) Br, (c) Pb and (d) Cs for Cs/FA/MA perovskite film with 2% H₂O.

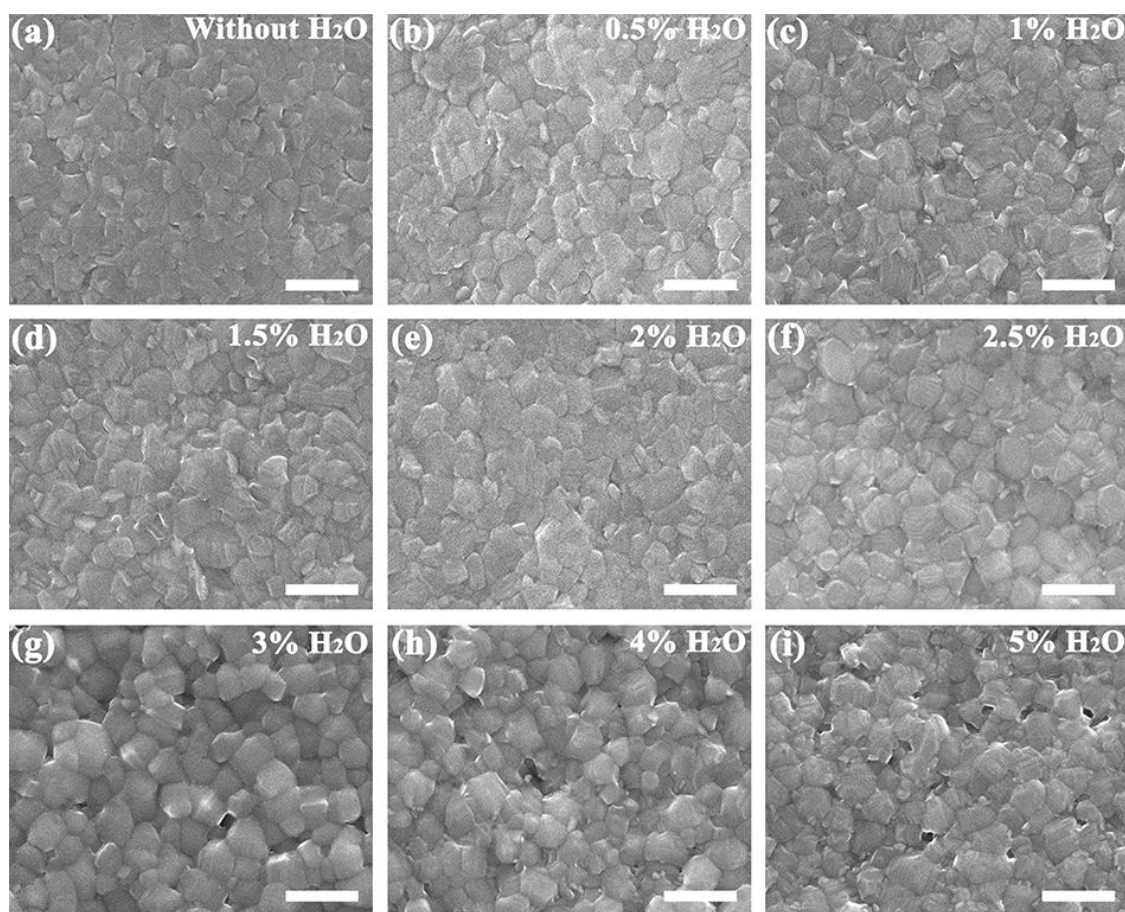


Figure S5. SEM images of 1st-A films with (a) 0%, (b) 0.5%, (c) 1%, (d) 1.5%, (e) 2%, (f) 2.5%, (g) 3%, (h) 4% and (i) 5% H₂O. The scale bar is 1 μm.

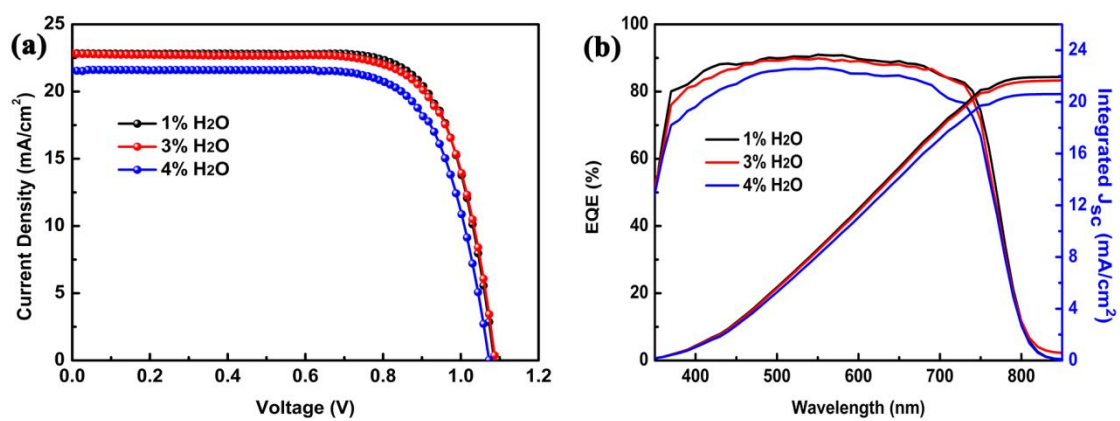


Figure S6. (a) J-V curves of the champion devices with 1%, 3% and 4% H₂O additive. (b) Corresponding EQE curves of the devices. The calculated J_{sc} are 21.9, 21.7 and 20.6 mA/cm², respectively.

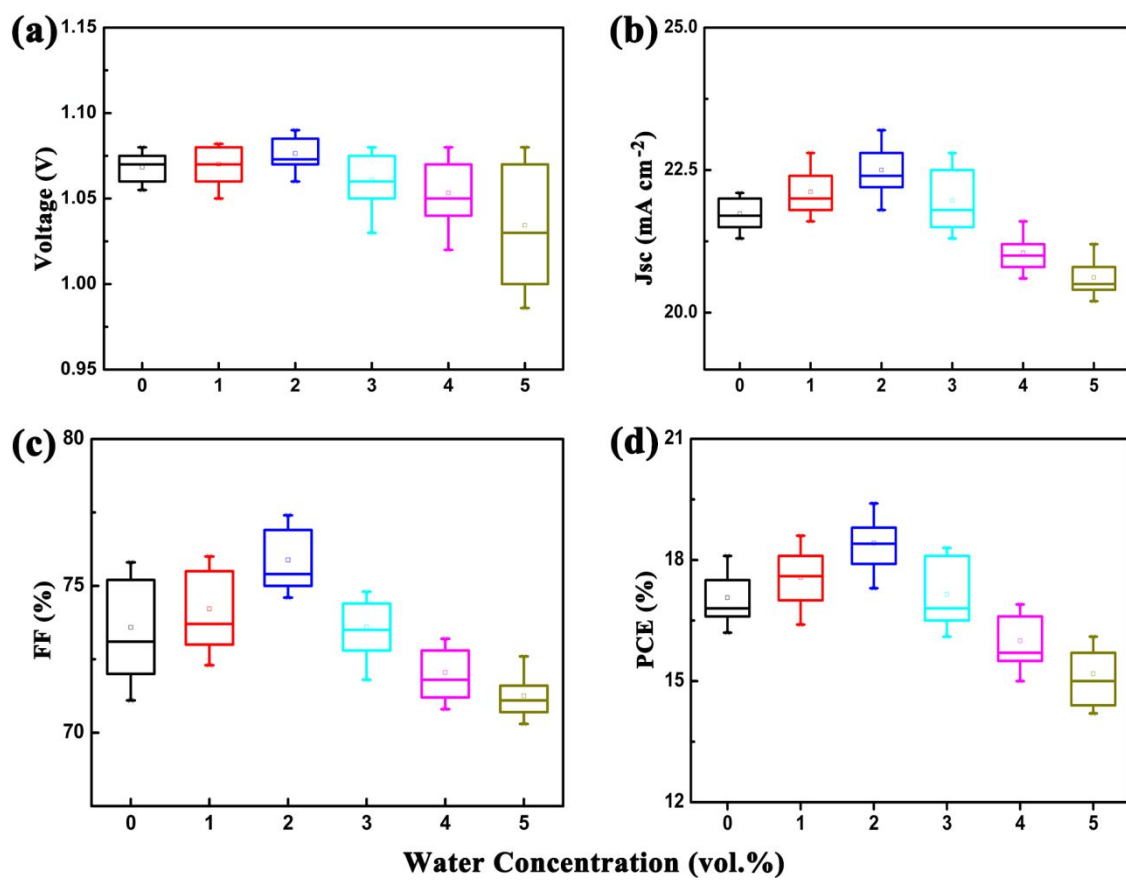


Figure S7. Photovoltaic parameters derived from devices with different water content. (a) short circuit current density, (b) open circuit voltage, (c) fill factor and (d) power conversion efficiency.

Table S1. Weight parameters of perovskites before and after TGA test.

Films	Water concentration	Before TGA (mg)	After TGA (mg)	Weight loss (mg)	Weight change (%)
1 st -A	W/O	4.93082	4.91606	0.01476	0.299
	2%	5.18569	5.14260	0.04309	0.831
	5%	7.75170	7.60569	0.14601	1.884
2 nd -A	W/O	4.53663	4.52180	0.01483	0.327
	2%	4.48953	4.47475	0.01478	0.329
	5%	6.61450	6.59044	0.02406	0.364

Table S2. Statistic of photovoltaic parameters of devices with different content of water.

Water content (vol. %)	Cells	Voc (V)	Jsc (mA/cm ²)	FF (%)	PCE (%)
0	A	1.08	22.1	75.8	18.1
	B	1.075	21.5	74.3	17.2
	C	1.07	21.8	75	17.5
	D	1.07	21.3	71.1	16.2
	E	1.06	22	71.8	16.8
	F	1.055	21.7	73.1	16.6
1	A ₁	1.082	22.8	75.5	18.6
	B ₁	1.08	22.1	76	18.1
	C ₁	1.078	22.4	73	17.6
	D ₁	1.07	22	74.8	17.7
	E ₁	1.06	21.8	73.7	17
	F ₁	1.05	21.6	72.3	16.4
2	A ₂	1.09	22.4	76.9	18.8
	B ₂	1.085	22.6	76.1	18.7
	C ₂	1.08	23.2	77.4	19.4
	D ₂	1.073	22.8	75.4	18.4
	E ₂	1.07	22.2	74.6	17.9
	F ₂	1.06	21.8	74.9	17.3
3	A ₃	1.08	22.8	74.3	18.3
	B ₃	1.075	22.5	74.8	18.1
	C ₃	1.07	21.8	73.5	17.1
	D ₃	1.06	21.3	74.4	16.8
	E ₃	1.05	21.9	71.8	16.5
	F ₃	1.03	21.5	72.8	16.1
4	A ₄	1.08	21.6	72.5	16.9
	B ₄	1.07	21.2	73.2	16.6
	C ₄	1.06	21.1	72.8	16.3
	D ₄	1.05	20.8	71.8	15.7
	E ₄	1.04	21	70.8	15.5
	F ₄	1.02	20.6	71.2	15
5	A ₅	1.08	20.6	72.6	16.1
	B ₅	1.07	20.8	70.7	15.7
	C ₅	1.04	21.2	71.2	15.7
	D ₅	1.03	20.5	71.1	15
	E ₅	1	20.2	70.3	14.2
	F ₅	0.986	20.4	71.6	14.4