

Electronic Supporting Information

High efficiency stable inverted perovskite solar cells without current hysteresis

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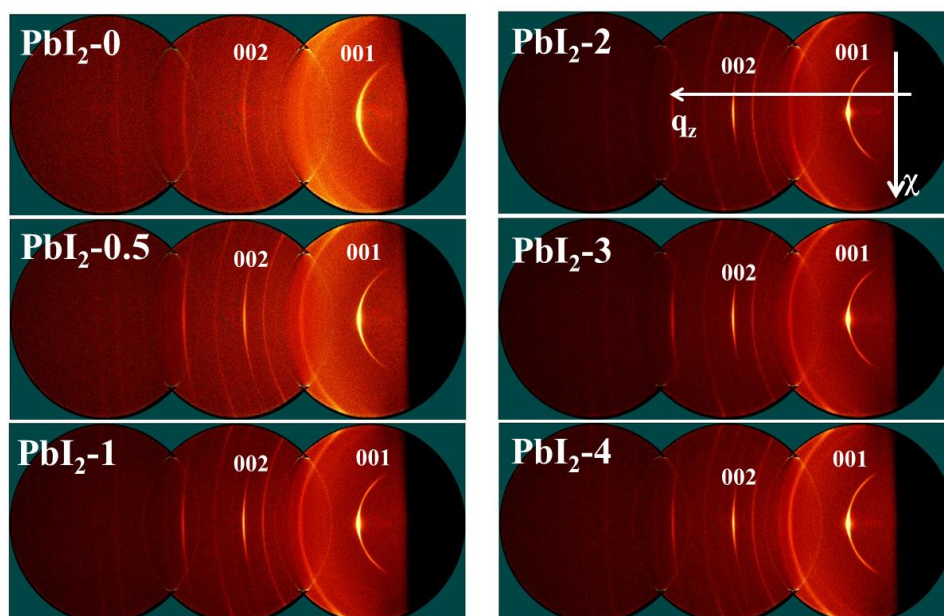


Figure S1: The original 2D GIXRD data.

Table S1: the peak intensity of (001) plane and the crystalline domain size of PbI₂ films

PbI ₂ film	Water content (vs DMF)	Intensity (cps/s)	Domain size (Å)
PbI ₂ -0	0	40.2	150
PbI ₂ -0.5	0.5 vol%	157	206
PbI ₂ -1	1 vol%	309	230
PbI ₂ -2	2 vol%	316	253
PbI ₂ -3	3 vol %	304	237
PbI ₂ -4	4 vol%	245	225

The original 2D GIXRD data displayed in Figure S1 clearly reveal the relative crystallinity of PbI₂ film prepared from the precursor solution containing various amount of water. The corresponding (001) peak intensity and the crystalline domain size calculated from the peak width of (001) diffraction were summarized in Table S1. All PbI₂ films show prefer orientation (along the χ axis) with their (001) planes perpendicular to the surface of the substrate. PbI₂-2 has the highest crystallinity and domain size and both values are very close to those of PbI₂-1 and PbI₂-3.

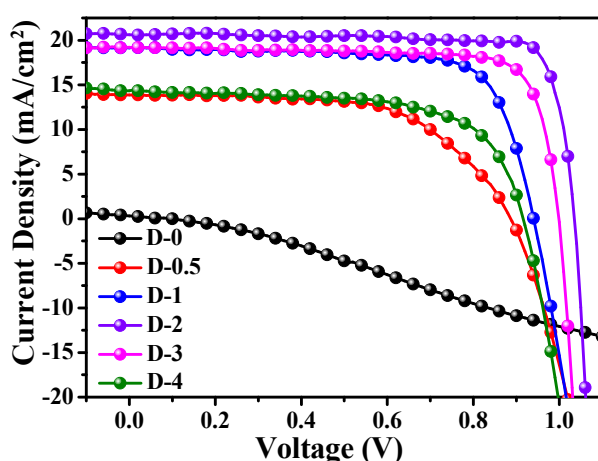


Figure S2: The I - V curves of the inverted perovskite solar cells based on perovskite films fabricated with two-step method with various H₂O content in PbI₂/DMF solution.

The I - V curves (shown in Figure S2) clearly demonstrated that the crystallinity and morphology of perovskite films are very important for the photovoltaic performance of the corresponding cells.

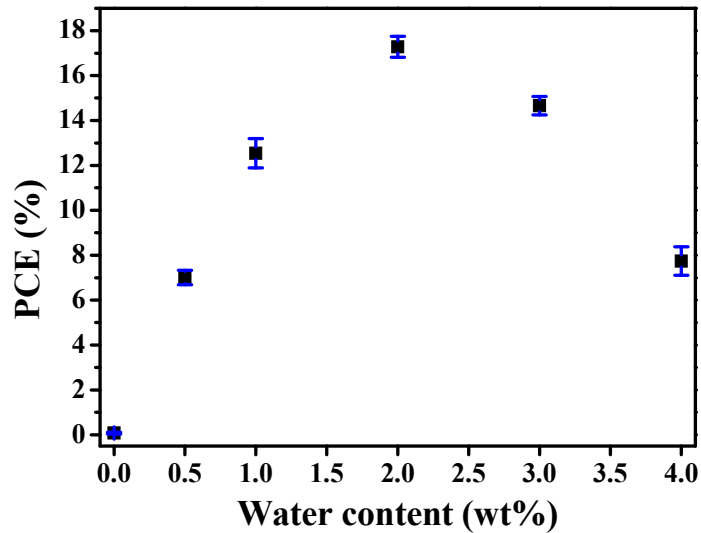


Figure S3: The efficiency statistical of cells fabricated with various amount of H₂O added in PbI₂/DMF precursor solutions.

The error bars were calculated by Equation (1) and the number of the samples is 20.

$$SD = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2} \quad \text{Equation (1)}$$

SD: standard deviation; n: number of samples

x_i : individual value; \bar{x} : average value

The derivation of the efficiency for 20 cells is small suggesting that the device fabrication method reported in this paper is a controllable method, therefore the efficiencies of the resulting cells are reproducible.

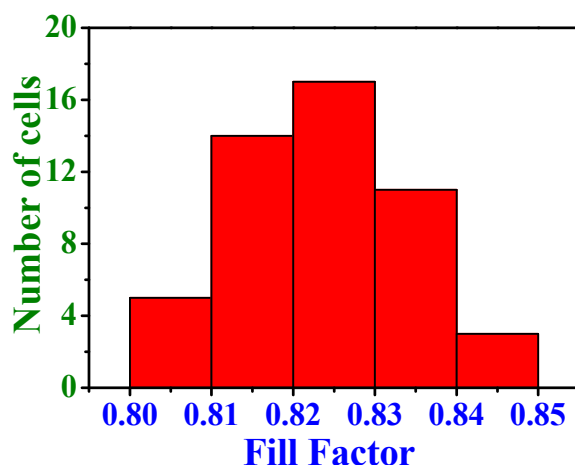


Figure S4: The histograms of FF for 50 cells prepared with 2 wt% H₂O in PbI₂/DMF precursor solutions.

Figure S4 illustrated the histograms of FF based on 50 devices. The FF of the inverted perovskite solar cells prepared using the method reported in this paper is very reproducible; the deviation is less than 10% for 50 cells.

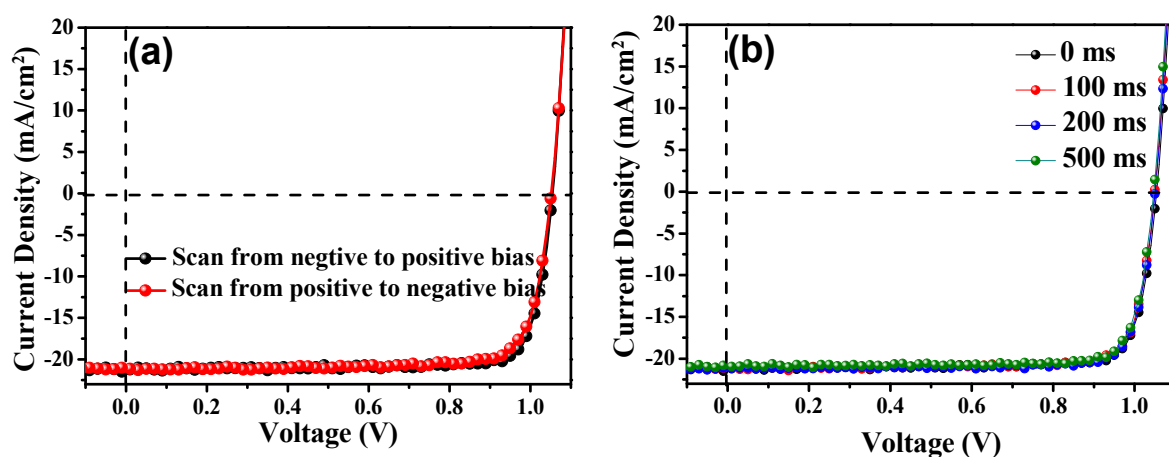


Figure S5: The I-V curves of the inverted perovskite device (a) scanned at two directions. (b) scanned with various delay times (delay time means the time between two data points, we take a datum every 0.01V).

The inverted perovskite solar cells fabricated with the method reported in this paper show no current hysteresis. The rate used for the scan with 0 sec delay time is 1.0 V/sec and one datum recorded every 0.01 V. In other words when the delay time is 500 ms and the scan range is 1.2 V, it takes 60 sec to record the $I-V$ curve.

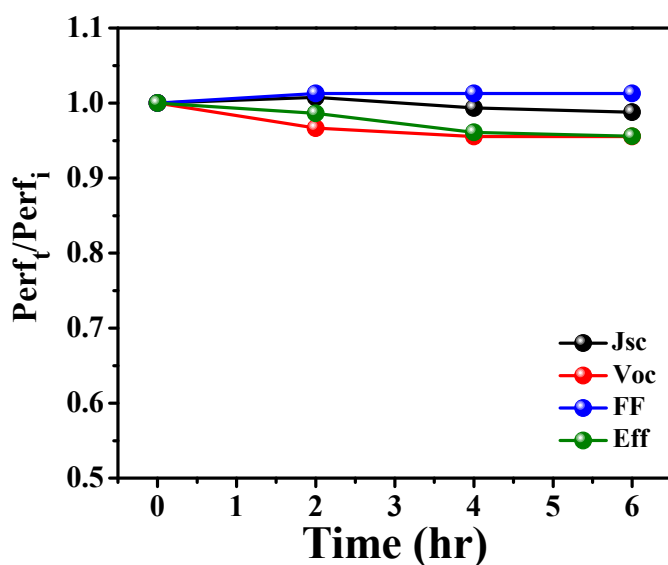


Figure S6: The variation of the photovoltaic performance (Perf) vs time for the inverted cell under the illumination of AM 1.5G simulated Sun light (100 mWcm^{-2}). Perf_i : initial value; Perf_t : the value at time t (hr.).

The device is stable under illuminating with AM 1.5 G (100 mWcm^{-2}) light. The efficiency decreases *ca.* 4% gradually in the first 4 hours and then stabilizes up to 6 hours (the test time).

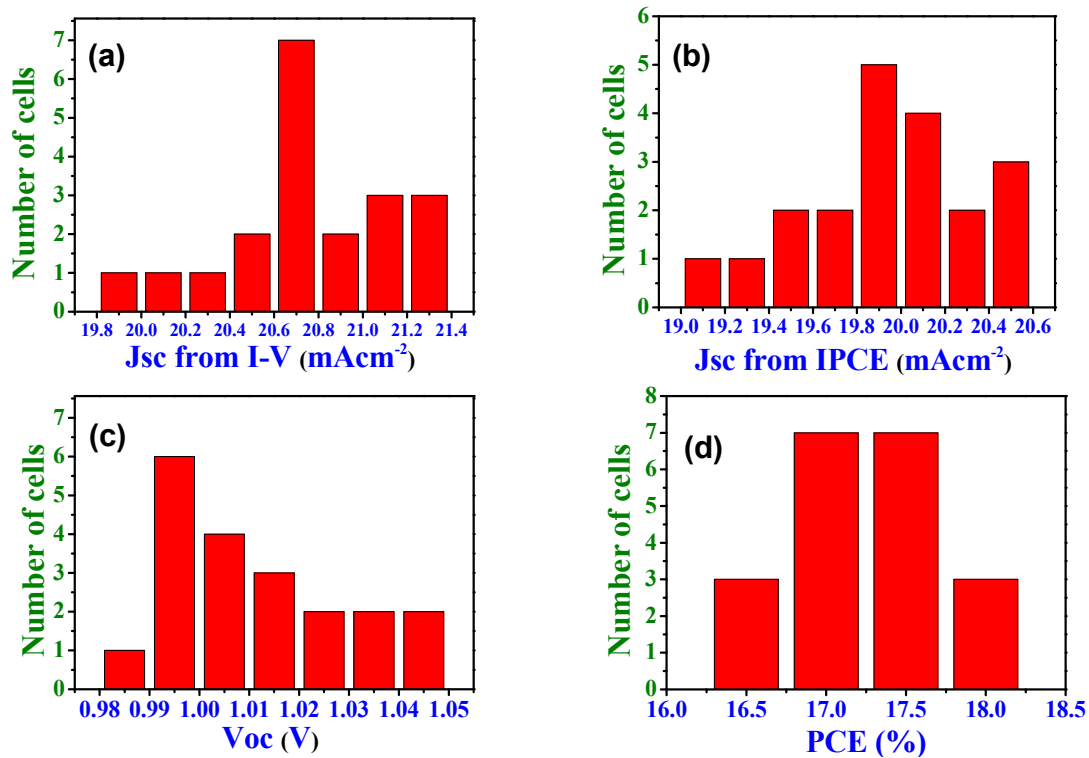


Figure S7: The histograms of (a) Jsc from I-V curves, (b) Jsc from integrated IPCE curves, (c) Voc, and (d) PCE for 20 cells fabricated (during 2 months period) with 2 wt% H₂O in PbI₂/DMF precursor solutions..

Table S2: Mean values, standard deviation (STD) and quartile deviation analysis of short-circuit current density, open-circuit voltage, fill factor, power conversion efficiency, and integrated current density (from IPCE) for 20 cells fabricated with 2 wt% H₂O in PbI₂/DMF precursor solutions.

Sample number	J _{sc} (mA/cm ²)	V _{oc} (V)	FF	PCE (%)	Integrated Current Density (from IPCE, mA/cm ²)
1	20.6	1.03	0.85	18	19.8
2	20.8	1.04	0.80	17	19.9
3	20.4	1.04	0.80	17	19.5
4	20.8	0.99	0.81	16	20.1
5	20.7	1.02	0.81	17	19.8
6	20.4	1.03	0.81	17	19.5
7	20.7	1.01	0.82	17	19.8
8	20.5	0.98	0.82	16	19.7
9	20.9	1.00	0.82	17	20.2
10	20.7	1.01	0.82	17	19.7
11	20.7	1.03	0.82	17	19.8
12	20.1	0.99	0.82	16	19.3
13	20.8	0.99	0.83	17	20.0
14	20.0	0.99	0.83	16	19.1
15	21.2	1.01	0.82	18	20.3
16	21.3	0.99	0.83	18	20.5
17	21.3	1.00	0.83	18	20.5
18	21.2	0.99	0.84	18	20.2
19	21.1	1.00	0.84	18	20.1
20	21.3	1.00	0.84	18	20.5
Mean	20.8	1.01	0.82	17	19.9
STD	0.4	0.02	0.01	0.75	0.4
1 st Quartile Q1	20.5	0.99	0.81	17	19.7
3 rd Quartile Q3	21.1	1.02	0.83	18	20.2
Interquartile Q3-Q1	0.6	0.03	0.02	1.0	0.5
Q1-k(Q3-Q1), k=0.5	20.2	0.98	0.80	16.5	19.5
Q3+k(Q3-Q1), k=0.5	21.4	1.04	0.84	18.5	20.5
Q1-k(Q3-Q1), k=1.0	19.9	0.96	0.79	16	19.2
Q3+k(Q3-Q1), k=1.0	21.7	1.05	0.85	19	20.7

The standard and expanded Uncertainties (combined the random and systematic errors) in measuring the efficiency are $\pm 4.0\%$ and $\pm 8.0\%$, respectively as the data listed in Table S5 and the explanations below the table. As the statistical (quartile deviation analysis) point of view, none of the efficiency data listed in Table S2 is an outlier (outlier means non-reasonable datum). If the measuring uncertainties (Table S4 and Table S5) were also concerned, the derivations of all

photovoltaic parameters are within the experimental error. In other words, the photovoltaic data of the 20 devices suggested that the devices are reproducible.

Table S3: The Imp, Vmp, spectrum mismatch (MM), Intensity of Irradiance (L) and mask area (A) of a reference diode measured 10 times.

item	Current at maximum power Imp (mA)	Voltage at maximum power Vmp (V)	Spectrum Mismatch (MM)	Intensity of Irradiance (L, mWcm ⁻²)	^c Mask area (A, cm ²)
1	0.6255	0.338	0.983	99.7	0.100
2	0.6332	0.333	0.986	100.4	0.099
3	0.6353	0.331	0.983	100.2	0.101
4	0.6388	0.329	0.981	99.9	0.099
5	0.6279	0.335	0.980	100.2	0.100
6	0.6284	0.335	0.981	100.3	0.101
7	0.6283	0.335	0.983	100.2	0.100
8	0.6282	0.335	0.980	99.9	0.099
9	0.6254	0.336	0.981	100.2	0.099
10	0.6295	0.334	0.981	100.3	0.101
^a Mean± absolute standard deviation	0.6301 ±0.0044	0.334 ±0.003	0.982 ±0.002	100.1 ±0.2	0.100 ±0.001
^b Mean± relative standard deviation (%)	0.6301 ±0.70%	0.334 ±0.9%	0.982 ±0.2%	100.1 ±0.2%	0.100 ±1.0%

a: The absolute standard deviation was calculated using equation (1) showing below the Figure S3.

b: The relative standard deviation was calculated by absolute standard deviation divided by mean value ×100%..

c, The area of the mask was defined with a close polyline to polygon under a microscope.

It takes 5~ 35 minutes to measure each type of data listed in Table S3. The times are much longer than the time we used to measure our test cells.

Table S4: Detailed measurement uncertainty estimation budget.

Item	Source of Measurement Uncertainty	Type A (Random) Standard Uncertainty (%) ^[1]	Type B (Systematic) Standard Uncertainty (%) ^[2]	Combined Standard Uncertainty (%) ^[3]	Note
1	Calibration of Secondary Reference Cell (RC)	0.0	0.75	0.75	[a]
2	Spectrum Mismatch factor (MMF)	0.2	2.35	2.36	[b]
3	Spatial Non-Uniformity of Irradiance	0.0	1.51	1.51	[c]
4	Instability of Irradiance	0.2	1.36	1.37	[d]
5	Measured Current of Reference Cell and Sample	0.70	0.37	0.79	[e]
6	Measured Voltage of Sample (within 25 ± 2 oC)	0.9	0.59	1.08	[f]
7	Uncertainty in Area Measurement of Sample	1.0	1.00	1.41	[g]

[1] The type A (random) standard uncertainty (%) was estimated by repeatedly (10 times) measurements using a silicon cell. The results were summarized in Table S3.

[2] The type B (Systematic) standard uncertainty (%) was estimated by using information (specification) of facility provided by manufacturer and periodically inspection/calibration.

[3] The combined standard uncertainty (%) is calculated with the combination of type A (random) standard uncertainty (%) and type B (systematic) standard uncertainty (%) according to ISO-GUM (JCGM 100:2008 - BIPM; Evaluation of measurement data — Guide to the expression of uncertainty in measurement).

[a] Current of the reference cell calibrated by TERTEC.

[b] 10 times measurements of spectrum mismatch factor dominated by repeatedly measuring EQE spectrum of the sample (SD (%) = 0.2%) and calibration of spectra-radiometer (2.35% from 300 nm to 800 nm).

[c] Maximum difference in irradiance intensity between the reference cell and sample (due to the discrepancy in area).

[d] 10 measurements of lamp (solar simulator) intensity using a silicon monitor cell (SD (%) = 0.2%), and long-term stability (more than 1 day) of solar simulator (1.36%).

[e] 10 measurements of current at maximum power for a silicon cell (SD (%) = 0.70%), and current calibration of IV tester (0.37%).

[f] 10 measurements of voltage at maximum power for a silicon cell (SD (%) = 0.9%), voltage calibration of IV tester (0.06 %), and calibration of thermometer (T-type thermocouple) (0.58%).

[g] 10 measurements of mask area (SD (%) = 1.0%), and the calibration of microscope with block gauge (1.00%).

Table S5: Combined^[1] standard measurement uncertainty and expanded uncertainty

Description		Standard Uncertainty (%) ^[2]	Expanded Uncertainty (%) ^[3]
U_{Isc}	Combined measurement uncertainty in Isc of Sample (to combine the uncertainty from listed item 1 to 5 of Table S4)	3.3	6.6
U_{Jsc}	Combined measurement uncertainty in Jsc of Sample (to combine the uncertainty of Isc and area (item 7 of Table S4)	3.6	7.2
U_{Voc}	Combined measurement uncertainty in Voc of Sample (listed item 6 of Table S4)	1.1	2.2
U_{Pmax}	Combined measurement uncertainty in Pmax of Sample (to combine the uncertainty of Isc and Voc listed above)	3.5	7.0
$U_{Eff}^{[4]}$	Combined measurement uncertainty in Efficiency (to combine uncertainty of Pmax, Irradiance intensity (item 4 in Table S4) and area (item 7 in Table S4))	4.0	8.0
U_{FF}	Combined measurement uncertainty in FF (to combine uncertainty of Isc, Voc and Pmax listed above)	4.9	9.8

[1] The combined standard uncertainty (%) is calculated with the combination of type A (random) standard uncertainty (%) and type B (systematic) standard uncertainty (%) according to ISO-GUM (JCGM 100:2008 - BIPM; Evaluation of measurement data — Guide to the expression of uncertainty in measurement).

[2] Standard Uncertainty is estimated with coverage factor (k) = 1 for 68% confidence level.

[3] Expanded Uncertainty is estimated with coverage factor (k) = 2 for 95% confidence level.

[4] The standard uncertainty of efficiency is propagated as $\Delta Eff (\%) = \sqrt{(3.5)^2 + (1.37)^2 + (1.41)^2} = 4.0$.