COMMUNICATION

Potassium Stearate Doped PEDOT: PSS Improves the Performance of Inverted Perovskite Solar Cells

Supporting Information

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Experiments

Materials

Lead iodide (PbI_2,>99.99%) and formamidine iodide (FAI, 99.90%) were purchased from Liaoning Youxuan Technology (China). Lead chloride ($PbCl_2$,>99.99%), methyl ammonium iodide (MAI), PEDOT:PSS (1.3%-1.7%), [6,6]-phenylC_{61} butyrate methyl ester ($PC_{61}BM$, 99%), bath copper (BCP,>99%) and silver (Ag, 99.99%) were purchased from Xi'an Polymer Light Technology Corp (China). N. N-dimethylformamide (DMF, 99.9%), dimethyl sulfoxide (DMSO, 99.7%), chlorobenzene (CB, 99.90%), ethanol (He, 99.90%) purchased from Beijing Bailingwei (China).

Sample preparation

The devices with the structure of ITO/K-PEDOT: PSS/Perovskite/PCBM/BCP/Ag were fabricated. The perovskite precursor was prepared by mixing MAI (200.3 mg), PbI_2 (580.8 mg), $PbCl_2$ (38.9 mg), and FAI (24 mg) in DMSO (100 μL) and DMF (900 μL) and stirring overnight at room temperature. Firstly, deionized water and Decom 90 (vol ratio=4:1) were added to the ITO (15 Ω sq^{-1}) substrate, and cleaned in a 50 ℃ ultrasound machine. The deionized water was sonicated three times. Then, PEDOT:PSS (40 μl) solutions doped with different concentrations of potassium stearate were spun onto the cleaned ITO substrate at 6000 rpm for 40 s, and the film was annealed at 130 ℃ for 20 min. After cooling, the perovskite precursor solution (35 μL) was spin-coated on PEDOT: PSS layer at 400 rpm for 3s and 4000 rpm for 30 s. During spin coating, CB (80 μL) was dropped onto the spinning substrates. Then, the perovskite-coated film was heated at 50 ℃ for 2 min and then 85 ℃ for 30 min. After cooling to room temperature, take 35 μl of 20 mg/mL PCBM solution dissolved in CB and spin it onto the perovskite film at 5000 rpm for 30 s. Then, transfer the substrate out of the glove box and air anneal for 30 min before transferring it into the glove box. Take 35 μl of 0.5mg/mL BCP solution dissolved in ethanol and spin coat it on the PCBM membrane at a speed of 2000 rpm for 30 s. Finally, the substrate was moved to a vacuum chamber and a 60 nm silver (Ag) electrode was deposited using thermal evaporation.

Device characterization

The current density voltage (J-V) characteristics are measured by Keithley 2400 source measuring instrument under 100mW/cm^2 analog light (AM 1.5G) in the glovebox The roughness, crystal and morphology characteristic of the film was investigated by Atomic force microscope (AFM, CSPM5500), X-ray diffraction system (XRD, Rigaku D/MAX2500PC)) and field emission scanning electron microscopy (SEM, HITACHI Regulus8220) respectively. The absorption of perovskite thin films was tested using UV visible absorption spectroscopy (UV-8000S), and elemental studies were conducted using X-ray photoelectron spectroscopy (XPS Thermo ScientificTM NexsaTM). The steady-state photoluminescence (PL) spectra were measured with LS-50B

luminescence spectrometer (Perkin-Elmer). Electrochemical impedance spectroscopy (EIS) is obtained by applying a bias voltage of 0.8V in the dark (model 660D, Shanghai Chenhua Instrument Co., Ltd., China)

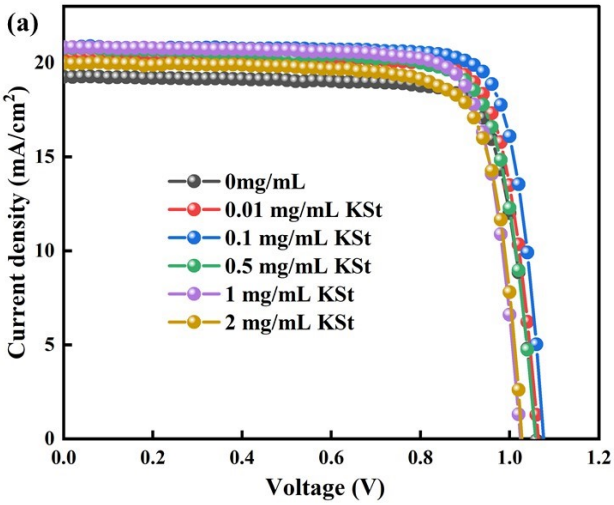

Fig.S1 (a) J-V curve of the 0 mg/mL 0.01 mg/mL 0.1 mg/mL 0.5 mg/mL 1 mg/mL and 2 mg/mL devices

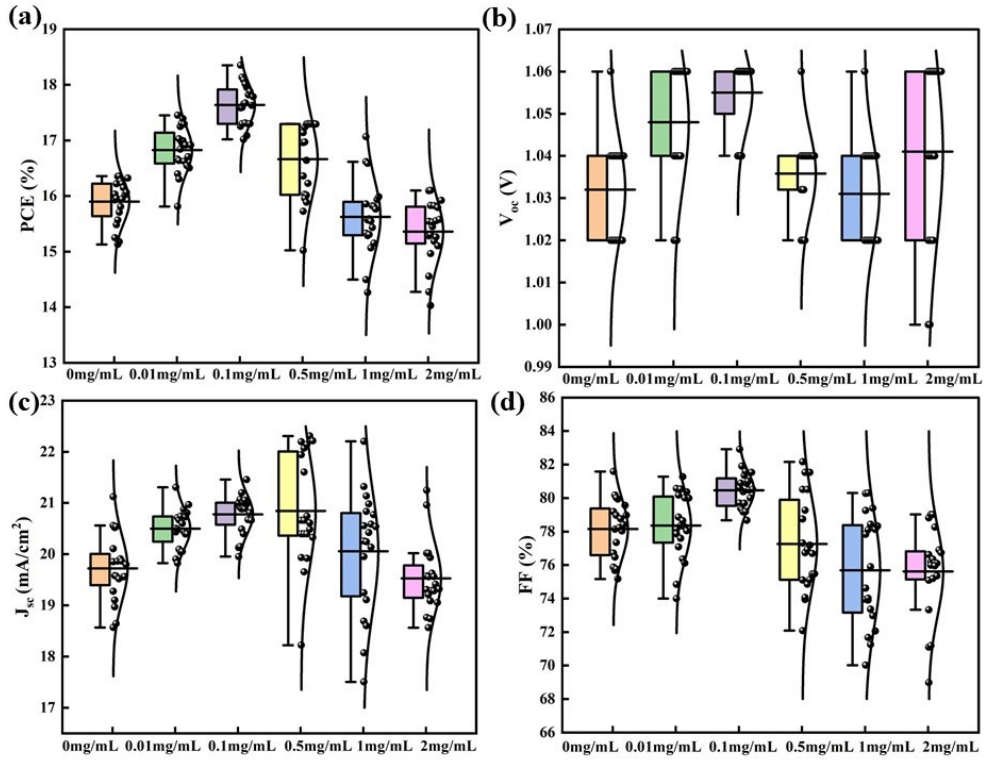

Fig.S2 Statistical analasis of the photovoltaic performance of 20 groups for devices with potassium stearate concentrations of 0 mg, 0.01 mg, 0.1 mg, 0.5 mg, 1 mg, and 2 mg

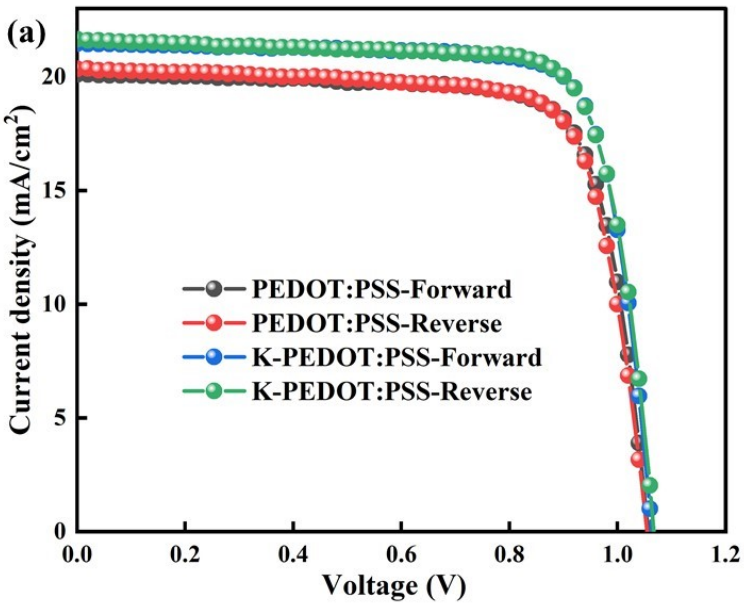

Fig. S3 (a)J-V hysteresis of the optimal PSCs with PEDOT:PSS and K-PEDOTl:PSS ETLs under reverse and forward scans.

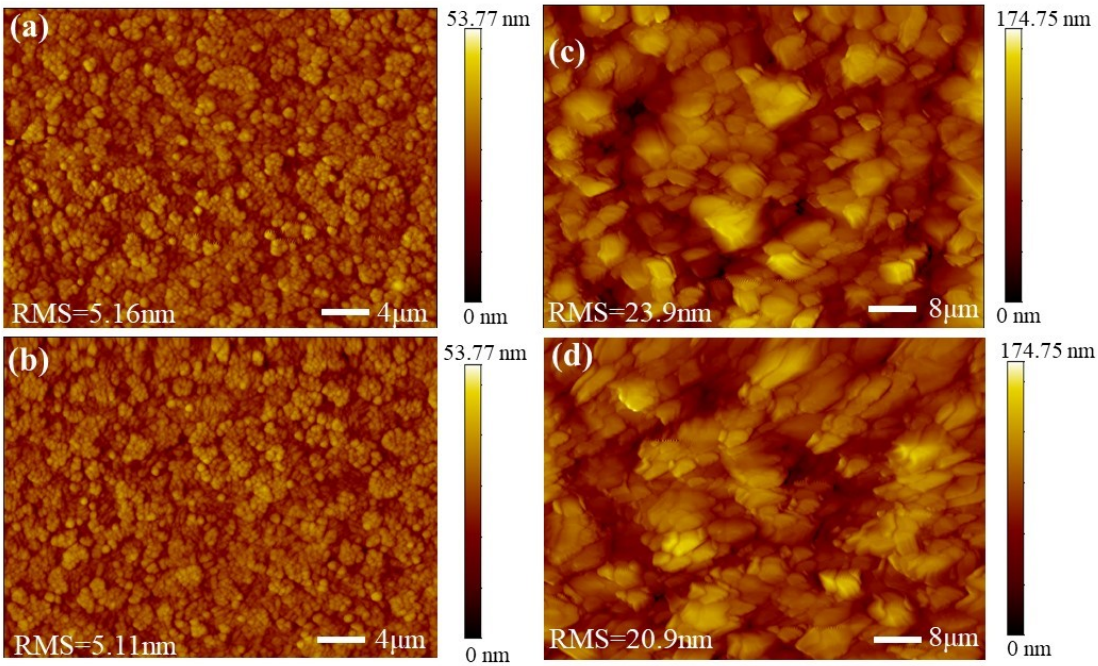

Fig.S4 (a) AFM image of ITO/PEDOT:PSS; (b) AFM image of ITO/K-PEDOT:PSS; (c) AFM image of ITO/PEDOT:PSS/Perovskite; (d) AFM image of ITO/K-PEDOT:PSS/Perovskite.

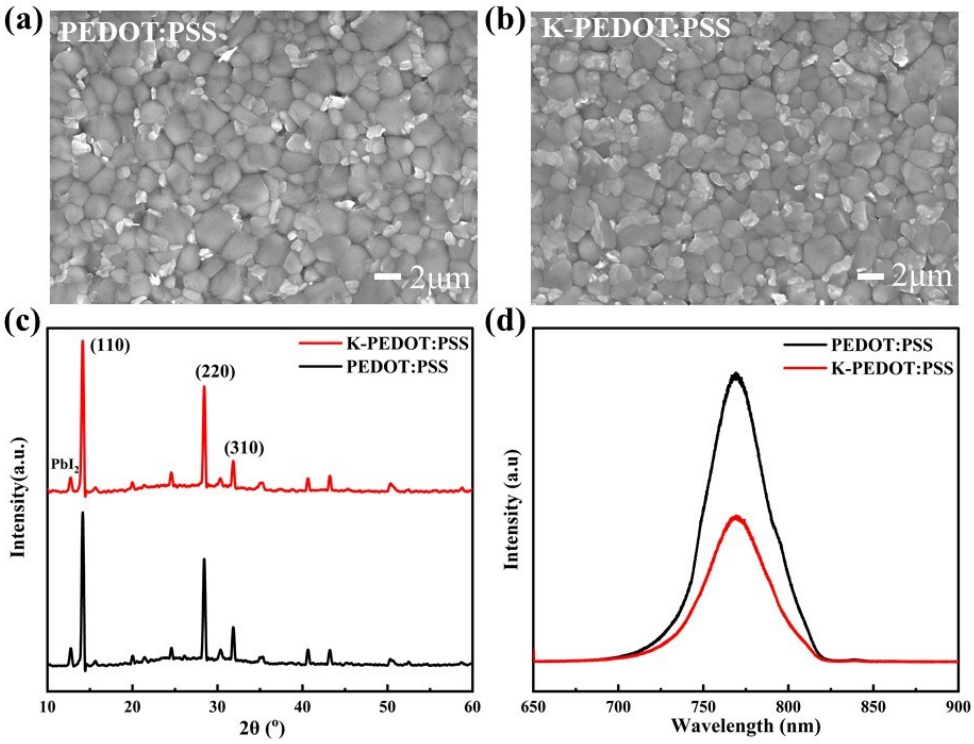

Fig.S5 SEM of (a) ITO/PEDOT:PSS/Perovskite and (b) ITO/K-PEDOT:PSS/Perovskite; (c) X-ray diffractometer; (d) Steady-state fluorescence spectrum

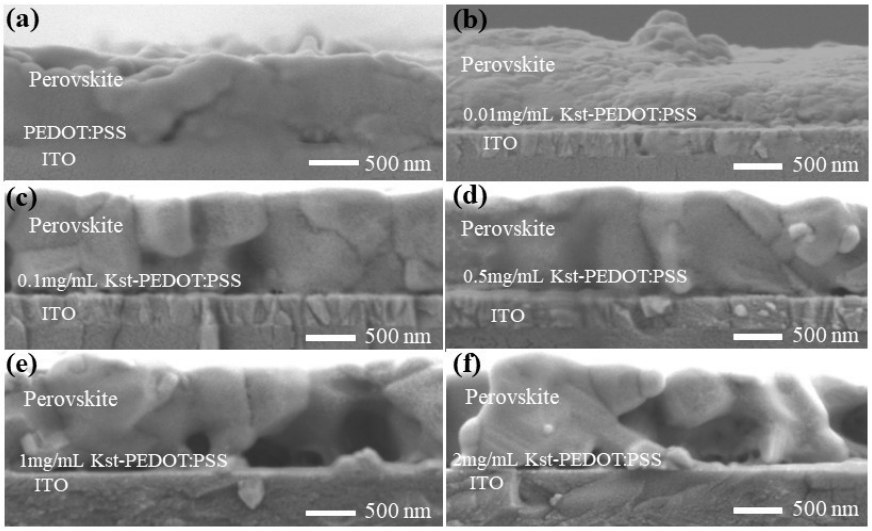

Fig. S6 Cross-sectional SEM of perovskite film coated on (a) ITO/PEDOT:PSS layer; (b-f) ITO/ Kst-PEDOT: PSS layer (Kst concentrations of 0 mg/mL 0.01 mg/mL, 0.1 mg/mL, 0.5 mg/mL, 1 mg/mL, and 2 mg/mL)

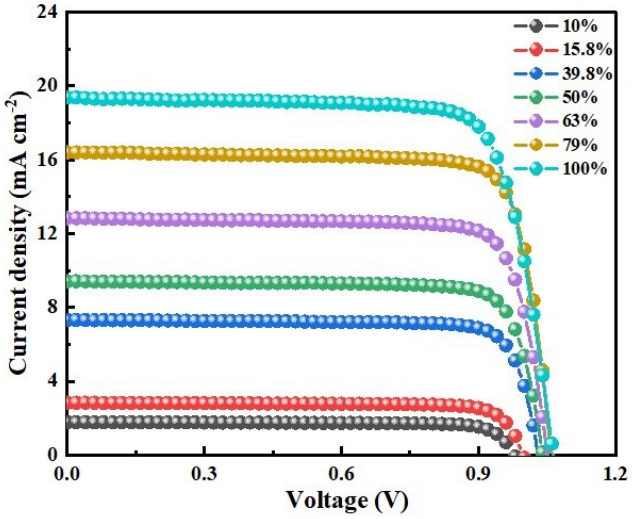

Fig.S7 The lighting intensity of the solar simulator is the J-V curve of 0.1 sun, 0.158 sun, 0.398 sun, 0.5 sun, 0.63 sun, 0.79 sun, and 1.0 sun

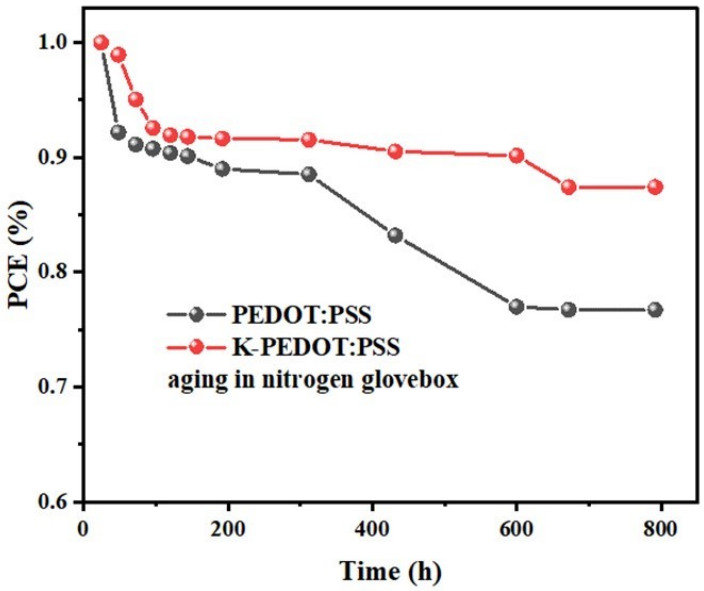

Fig.S8 The stability of PSCs with potassium stearate (0 and 0.1 mg/mL) doped in PEDOT:PSS.

Table S1 Device parameters of the 0 mg/mL 0.01 mg/mL 0.1 mg/mL 0.5 mg/mL 1 mg/mL and 2 mg/mL devices under AM 1.5G illumination at 100 mW/cm^2.

Device	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF (%)
0 mg/mL	1.04	19.27	16.35	81.58
0.01 mg/mL	1.06	20.43	17.45	80.56
0.1 mg/mL	1.06	20.88	18.35	82.91
0.5 mg/mL	1.04	20.40	17.29	81.53
1 mg/mL	1.02	20.84	17.07	80.30
2 mg/mL	1.02	20.02	16.09	78.82

Table S2 Statistical analysis of the photovoltaic performance of 20 groups for devices with potassium stearate concentrations of 0 mg/mL

No.	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF (%)
1	1.02	19.85	16.03	79.19
2	1.06	19.58	16.22	78.14
3	1.04	19.27	16.35	81.58
4	1.04	18.57	15.25	78.96
5	1.04	19.10	15.93	80.18
6	1.02	19.57	15.96	79.93
7	1.04	20.10	16.35	78.23
8	1.04	19.86	16.27	78.76
9	1.02	18.97	15.48	80.02
10	1.04	20.56	16.22	75.87

11	1.04	20.52	16.15	75.67
12	1.04	19.52	15.57	76.71
13	1.02	20.54	16.02	76.47
14	1.02	19.91	15.71	77.35
15	1.02	19.86	15.81	78.03
16	1.04	19.55	15.94	78.40
17	1.02	18.64	15.13	79.56
18	1.04	19.56	16.07	78.97
19	1.02	21.12	16.32	75.77
20	1.02	19.80	15.18	75.17

Table S3 Statistical analysis of the photovoltaic performance of 20 groups for devices with potassium stearate concentrations of 0.01 mg/mL

No.	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF (%)
1	1.06	20.43	17.45	80.57
2	1.04	20.50	16.66	78.14
3	1.02	20.71	15.81	74.84
4	1.06	19.90	16.64	78.86
5	1.04	20.67	16.84	78.34
6	1.04	20.74	16.96	78.65
7	1.06	20.48	16.99	78.27
8	1.06	20.09	16.62	78.04
9	1.04	21.31	16.40	74.00

10	1.06	20.04	17.03	80.17
11	1.04	20.60	17.25	80.53
12	1.02	20.88	17.31	81.28
13	1.02	20.73	16.92	80.00
14	1.06	20.05	16.55	77.86
15	1.04	20.80	17.39	80.37
16	1.06	20.45	16.71	77.09
17	1.06	19.82	16.30	77.59
18	1.06	20.39	16.51	76.36
19	1.06	20.97	16.92	76.11
20	1.06	20.40	17.29	79.99

Table S4 Statistical analysis of the photovoltaic performance of 20 groups for devices with potassium stearate concentrations of 0.1 mg/mL

No.	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF (%)
1	1.04	20.97	17.59	80.62
2	1.04	20.91	17.59	80.89
3	1.06	20.88	18.35	82.91
4	1.06	20.89	17.65	79.70
5	1.06	20.89	18.14	81.91
6	1.06	21.00	17.67	79.38
7	1.06	21.07	17.95	80.38
8	1.06	20.97	18.09	81.36

9	1.06	21.20	17.82	79.30
10	1.06	20.67	17.88	81.59
11	1.06	21.01	17.63	79.17
12	1.06	21.06	17.79	79.69
13	1.06	20.13	17.25	80.87
14	1.06	20.15	17.30	81.00
15	1.06	19.95	17.02	80.47
16	1.06	21.46	18.01	79.19
17	1.04	20.81	17.31	80.00
18	1.06	20.49	17.09	78.67
19	1.04	20.40	17.29	81.53
20	1.04	20.66	17.30	80.51

Table S5 Statistical analysis of the photovoltaic performance of 20 groups for devices with potassium stearate concentrations of 0.5 mg/mL

No.	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF (%)
1	1.06	22.19	16.96	72.08
2	1.04	22.07	16.97	73.94
3	1.04	21.94	17.14	75.11
4	1.04	21.60	16.64	74.06
5	1.04	22.14	17.24	74.85
6	1.03	22.31	17.29	75.12
7	1.03	22.21	17.29	75.46
8	1.03	20.40	17.29	82.17

9	1.04	20.66	17.29	80.51
10	1.04	20.40	17.29	81.53
11	1.04	20.66	17.29	80.51
12	1.04	20.40	17.29	81.53
13	1.02	20.74	16.36	77.31
14	1.02	20.48	16.03	76.73
15	1.02	19.93	16.01	78.75
16	1.04	19.65	15.72	76.93
17	1.02	20.61	16.23	77.19
18	1.04	18.22	15.02	79.27
19	1.04	20.33	15.96	75.48
20	1.04	19.92	15.89	76.68

Table S6 Statistical analysis of the photovoltaic performance of 20 groups for devices with potassium stearate concentrations of 1 mg/mL

No.	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF (%)
1	1.02	20.55	16.62	79.25
2	1.02	20.26	16.59	80.27
3	1.02	19.25	15.33	78.10
4	1.02	20.84	17.07	80.30
5	1.02	19.11	15.29	78.43
6	1.02	22.20	15.86	70.02
7	1.04	20.24	15.57	73.95
8	1.02	21.32	15.59	71.67

9	1.04	20.98	15.55	71.25
10	1.04	20.59	15.82	73.91
11	1.02	21.13	15.81	73.36
12	1.04	20.77	15.76	72.97
13	1.04	20.54	15.93	74.61
14	1.04	20.42	15.30	72.06
15	1.02	20.14	15.99	77.83
16	1.02	19.95	15.06	74.02
17	1.04	18.69	15.43	79.39
18	1.06	17.50	14.50	78.13
19	1.04	18.60	15.15	78.32
20	1.04	18.07	14.26	75.90

Table S7 Statistical analysis of the photovoltaic performance of 20 groups for devices with potassium stearate concentrations of 2 mg/mL

No.	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF (%)
1	1.04	19.57	15.28	75.09
2	1.04	19.31	14.27	71.09
3	1.04	19.21	15.30	76.62
4	1.02	20.02	16.09	78.82
5	1.04	19.56	14.03	68.98
6	1.06	19.93	16.09	76.20
7	1.06	19.09	15.45	76.35
8	1.02	20.02	15.54	76.13

9	1.06	19.29	14.56	71.19
10	1.06	19.63	15.83	76.10
11	1.06	19.28	15.53	75.99
12	1.06	19.41	15.82	76.91
13	1.06	19.05	15.18	75.19
14	1.06	19.32	15.55	75.96
15	1.06	18.77	15.26	76.73
16	1.00	20.96	15.79	75.35
17	1.00	21.25	15.58	73.33
18	1.02	18.56	14.96	79.02
19	1.02	18.74	15.10	79.02
20	1.04	19.56	15.92	78.26

Table S8 Summary of the PCE of inverted PSCs based on $MAPbI_{3-x}Cl_x$ and PEDOT:PSS, and their corresponding treatment method.

HTL	Perovskite	ETL	Treatment method	PCE
PEDOT:PSS[This work]	$MAPbI_{3-x}Cl_x$	$PC_{61}BM$/BCP	Potassium Stearate - Doped PEDOT:PSS	16.35%#
KSt/PEDOT:PSS[This work]				18.35%
PEDOT:PSS	$MAPbI_{3-x}Cl_x$	PCBM/RhB101/ LiF	Water rinsing to obtain PEDOT:PSS monolayer	13.40%#
PEDOT:PSS monolayer				18%
PEDOT:PSS	$MAPbI_{3-x}Cl_x$	PCBM/BCP	Sodium Citrate-Doped PEDOT:PSS	15.05%#
sodium citrate-				18.39%

PEDOT:PSS				
PEDOT:PSS PEDOT:PSS/KCl	$MAPbI_3$	PCBM/BCP	KCl add into PEDOT:PSS solution	15.67%# 17.09%
PEDOT:PSS	$MAPbI_3$	PCBM/BCP	$Ti_3C_2T_x$-doped PEDOT:PSS	12.5%# 15.01%
PEDOT:PSS LiF/PEDOT:PSS	$MAPbI_{3-x}Cl_x$	C_{60}/BCP	Inserting LiF between ITO and PEDOT:PSS	16.01%# 18.18%
PEDOT:PSS GMS/PEDOT:PSS	$MAPbI_3$	PCBM/BCP	Monostearic glycerol ester as intermediate layer on PEDOT: PSS	14.82%# 17.29%
PEDOT:PSS CuSCN/PEDOT:PSS	$MAPbI_3$	PCBM/C_{60}/LiF	CuSCN-doped PEDOT:PSS	13.2%# 15.3%

represents the PCE of control device in their corresponding work.

Table S9 Summary of stability and PCE of inverted PSCs based on $MAPbI_{3-x}Cl_x$ and PEDOT: PSS.

HTL	Perovskite	Stability	PCE%
PEDOT:PSS[This work]	$MAPbI_{3-x}Cl_x$	70% after 700 h Under N_2 atmosphere in the glove box	16.35%#
KSt/PEDOT:PSS[This work]		87% after 700 h Under N_2 atmosphere in the glove box	18.35%
PEDOT: PSS	$MAPbI_{3-x}Cl_x$	60.4% after 28 day Under N_2 atmosphere in the glove box	15.2%#
DA-PEDOT: PSS		85.4% after 28 day Under N_2 atmosphere in the glove box	16.6%

PEDOT:PSS	$MAPbI_3$	90.4% after 6 day Under N_2 atmosphere in the glove box	15.67%[#]
KCl/PEDOT:PSS		95.0% after 6 day Under N_2 atmosphere in the glove box	17.09%
CuSCN/PEDOT:PSS	$MAPbI_3$	71% after exposure to N_2 for 175 h	15.3%
PEDOT:PSS	$MAPbI_3$	70% after 350 h Under N_2 atmosphere in the glove box	14.82%[#]
GMS/PEDOT:PSS		85% after 350 h Under N_2 atmosphere in the glove box	17.29%

[#] represents the PCE of control device in their corresponding work.