Supporting Information for

Alleviation of perovskite toxicity and inhibition of lead leakage for sustainable perovskite solar cells

MATERIALS AND METHODS

Materials

Cesium iodide (CsI, 99.99%) was purchased from Aladdin. Lead bromide ($PbBr_2$, 99.99%), anhydrous dimethyl sulfoxide (DMSO, 99.7%), diethanol amine (99%), titanium (IV) isopropoxide (99.9%), isopropanol (IPA, 99.5%), Rutin (99.8%), DB18C6(99.8%), chlorobenzene (CB, 99.9%) and ethanol (99.7%) were purchased from Macklin. Lead iodide (PbI_2, 99.99%) were obtained from Xi'an Yuri Solar Co., Ltd. Zinc powder, acetone, nitric acid, sulfuric acid, and hydrochloric acid were obtained from AR Guangzhou Chemical Reagent Factory. Commercial carbon paste was obtained from Shanghai MaterWin New Materials (MTW-CE-C-003, ≈10 Ω sq^{-1}). Fluorine-doped tin oxide coated (FTO) substrates with a sheet resistance of 14 Ω sq^{-1} were purchased from Pilkington. Cell Counting Kit-8 (CCK-8) was purchased from Dojindo Molecular Technologies, Inc. (Tokyo, Japan). The Clone9 cells and HK-2 cells were purchased from Fuheng Biotechnology Co. (Shanghai, China) and cultured in DMEM/F-12 (Dulbecco's Modified Eagle Medium/Nutrient Mixture F-12), supplemented with 10% fetal bovine serum (FBS) (Gibco, Thermo Fisher), 1% penicillin and incubated at 37 °C, 5% CO_2 and 95% humidified air for incubation. The RAW264.7 cells were kindly provided by Wuhan Pricella Biotechnology Co. and cultured in DMEM (Dulbecco's Modified Eagle Medium), supplemented with 10% fetal bovine serum (FBS) (Gibco, Thermo Fisher), 1% penicillin and incubated at 37 °C, 5% CO_2 and 95% humidified air for incubation. The cells were passaged every 1–2 days and used at 80%–90% confluence. Arabidopsis thaliana seeds were provided by the Laboratory of Traditional Chinese Medicine Resources Development and Utilization of Linyi University. Unless mentioned otherwise, all the materials and reagents were commercially purchased and used as received free of further purification.

Fabrication of PSCs

FTO was first etched with the desired pattern via zinc powder and hydrochloric acid and then consecutively washed with deionized water, acetone, isopropanol, and ethanol in an ultrasonic bath for 30 min, respectively, and finally treated with UV-ozone for

180 s. A compact titanium dioxide layer (c-TiO_2) was prepared by spin-coating a solution (0.5 M diethanol amine and 0.5 M titanium isopropoxide ethanol solution, respectively) at 7000 rpm for 30 s, and then annealed at 500 °C for 2 h in air. Prior to transferring the cool-down substrates into an N_2 glove box, the FTO/c-TiO_2 substrates were treated with UV-ozone for another 180 s. $CsPbI_2Br$ perovskite layer was deposited via a two-step thermal treatment process. Briefly, 80 μL of 1.2 M $CsPbI_2Br$ precursor solution containing 312 mg of CsI, 220 mg of $PbBr_2$ and 277 mg of PbI_2, dissolved in 1 mL DMSO was spin-coated onto FTO/c-TiO_2 substrate at 1000 rpm for 10 s and then 3000 rpm for 30 s. A hot flow of 100 °C was blown onto the substrate until the color of the film turned brown. The distance between the muzzle of hot-air gun (858D, DongGuan BuFan Electronics Co., LTD) and the substrate was ≈ 4 cm. The whole blowing process lasted ≈ 20 s. Afterward, the substrate was placed on a hotplate at 160 °C for 1 min and then at 270 °C for 10 min and cooled down to room temperature naturally. Subsequently, rutin and crown ether were dissolved in chlorobenzene to prepare solutions of varying concentrations. These solutions were then spin-coated onto the perovskite layer at 3000 rpm for 30 seconds, followed by annealing on a hotplate at 100°C for 5 min. Finally, the commercial carbon paste was bladed onto the perovskite film with an active area of 0.09 cm^2 and then dried at 200 °C for 2 min.

Characterizations

The morphologies were conducted by scanning electron microscopy (SEM, Regulus8600, JAPAN). X-ray photoelectron spectroscopy (XPS) spectra were measured via a RBD upgraded PHI-5000C ESCA system (Perkin Elmer) equipped with Mg Kα as the X-ray source (hv = 1253.6 eV). The crystallinity of perovskite films was determined by the X-ray diffraction (XRD, Bruker D8 ADVANCE) with Cu Kα (λ = 1.5406 Å) radiation at 40 kV and 40 mA. The optical absorption spectra of perovskite films were characterized by UV-vis spectrophotometer (UV-8000A) under the wavelength range of 300-800 nm. The steady-state photoluminescence (PL) spectra and time-resolved photoluminescence (TRPL) spectra were obtained on a FluoroMax-4 spectrofluorometer and a Horiba spectrometer under excitation wavelength of 410 and

470 nm, respectively. The external quantum efficiency (EQE) spectra of devices were obtained by a IPCE kit developed by Enli Technology Co., Ltd. with a standard Si crystalline solar cell as a reference. The current density-voltage (*J-V*) curves of solar cells were measured on an electrochemical workstation (CHI660E) under standard solar irradiation (Enli, Oriel Class A, AM 1.5G,100 mW cm^{-2}, calibrated by a standard silicon solar cell) equipped with 500 W Xenon lamp. The steady-state output of photocurrent and PCE were measured via an electrochemical workstation (CHI660E) under a certain bias. The electrochemical impedance spectroscopy (EIS) measurements and the Mott-Schottky plots, dark *J-V* curves were conducted on the CHI660E electrochemical workstation. The light stability was performed under constant irradiation by a LED lamp in the air. All the moisture durability were measured on the devices without encapsulation. The concentration of lead ions is tested by inductively coupled plasma spectrometer (ICP-MS EXPEC6000). Laser confocal microscopy (LeicaTCS SP8+LeicaAM TIRF MC) was used to detect the survival of fluorescently stained cells. Cell viability was measured by fluorescence microplate reader (synergyHTX). Cell viability was quantitatively determined using the CCK-8 assay. Three different cell types were seeded in 96-well plates and incubated for 24 hours at 37° C. Following this, CCK-8 solution was added to each well to indicate the presence of viable cells. The absorbance was measured at 450 nm using a microplate reader. The experiment was independently repeated three times, with three technical replicates for each group per experiment.

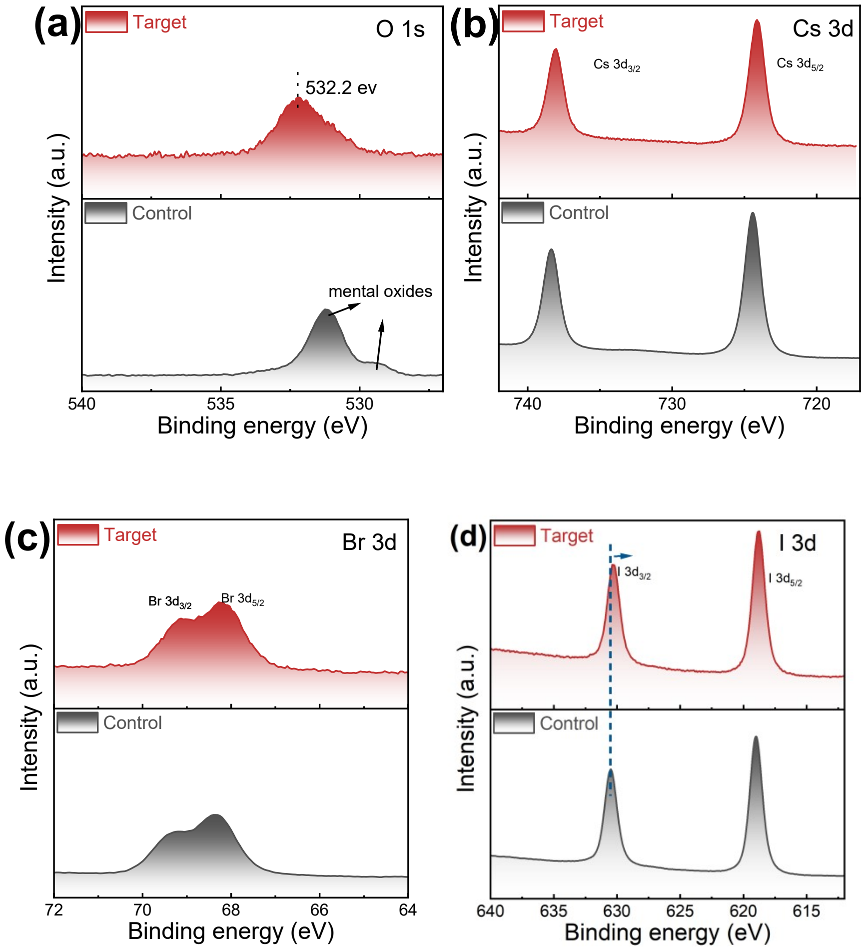

Figure S1. XPS spectra of (a) O 1s, (b) Cs 3d, (c) Br 3d, and (d) I 3d control and Rutin-modified perovskite films.

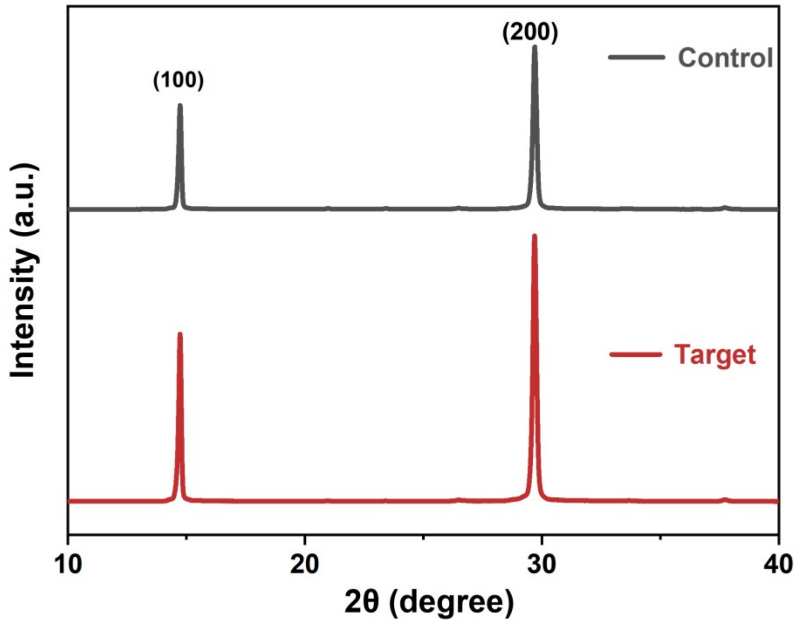

Figure S2. XRD patterns.

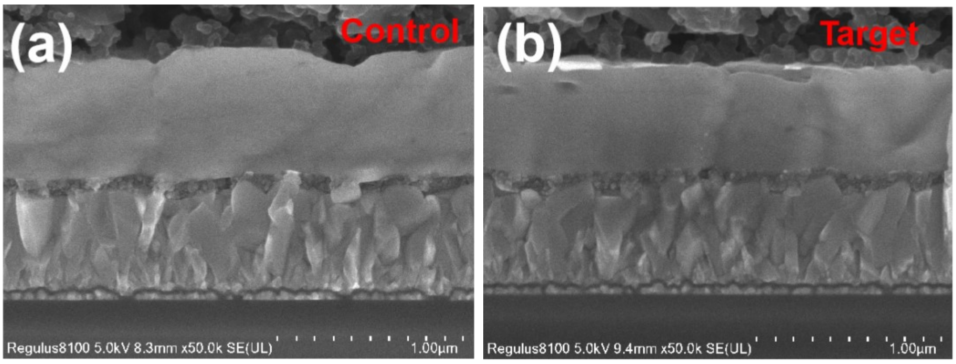

Figure S3. Cross-sectional SEM images of (a) control and (b) Rutin-treated $CsPbI_2Br$ films deposited on FTO/c-TiO_2 substrate.

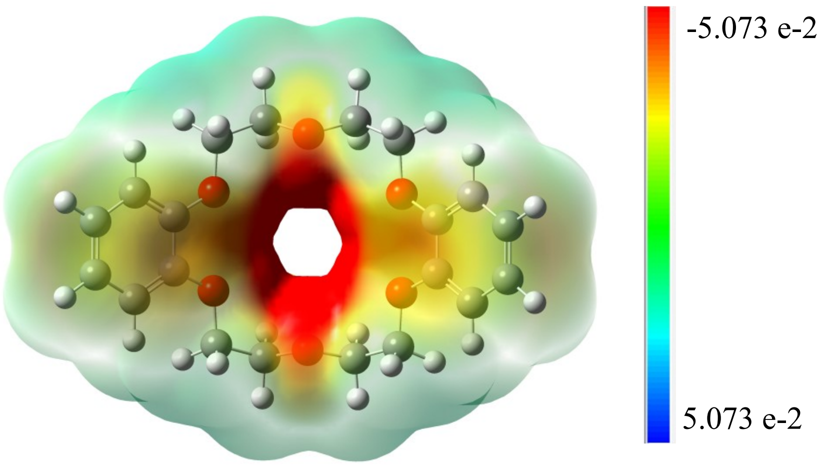

Figure S4. Electrostatic Potential of DB18C6.

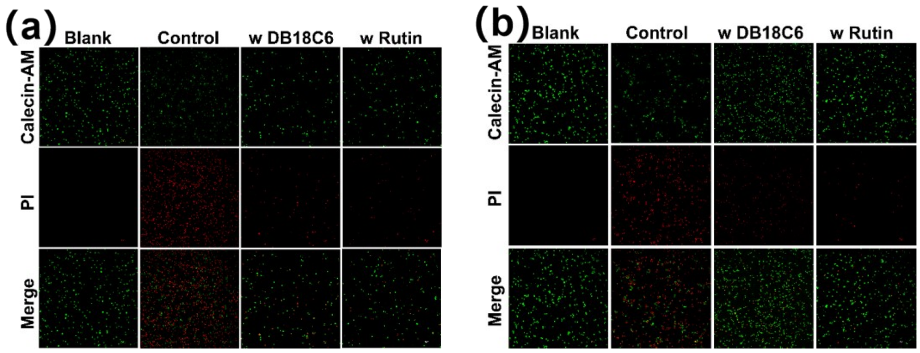

Figure S5. Laser confocal images of (a) stained RAW cells and (b) HA-2 cells in different mediums.

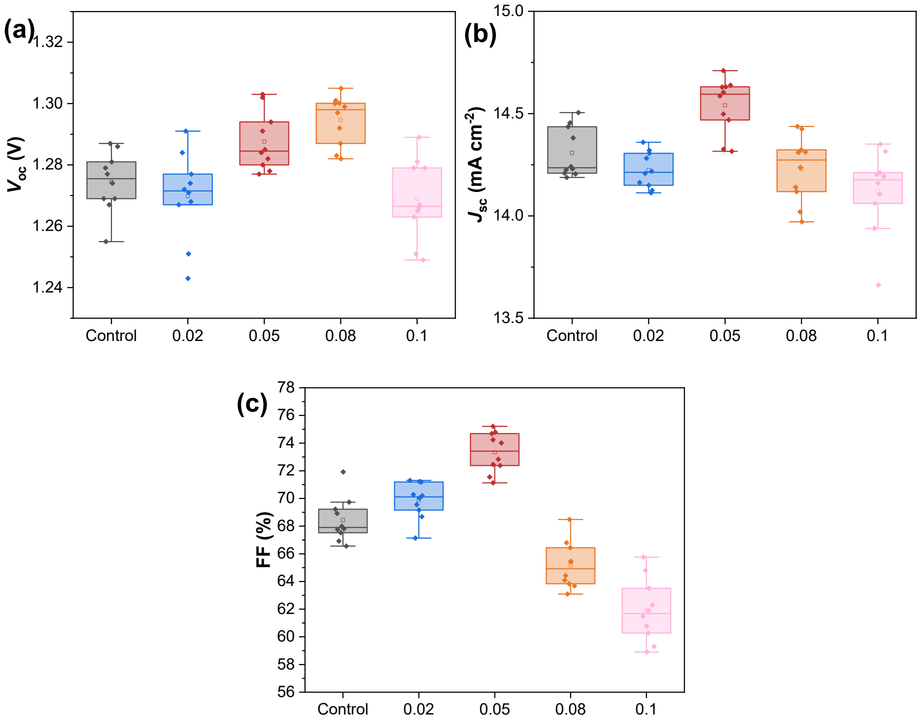

Figure S6. (a-c) V_{OC}, J_{SC} and FF values of $CsPbI_2Br$ PSCs with different Rutin concentrations.

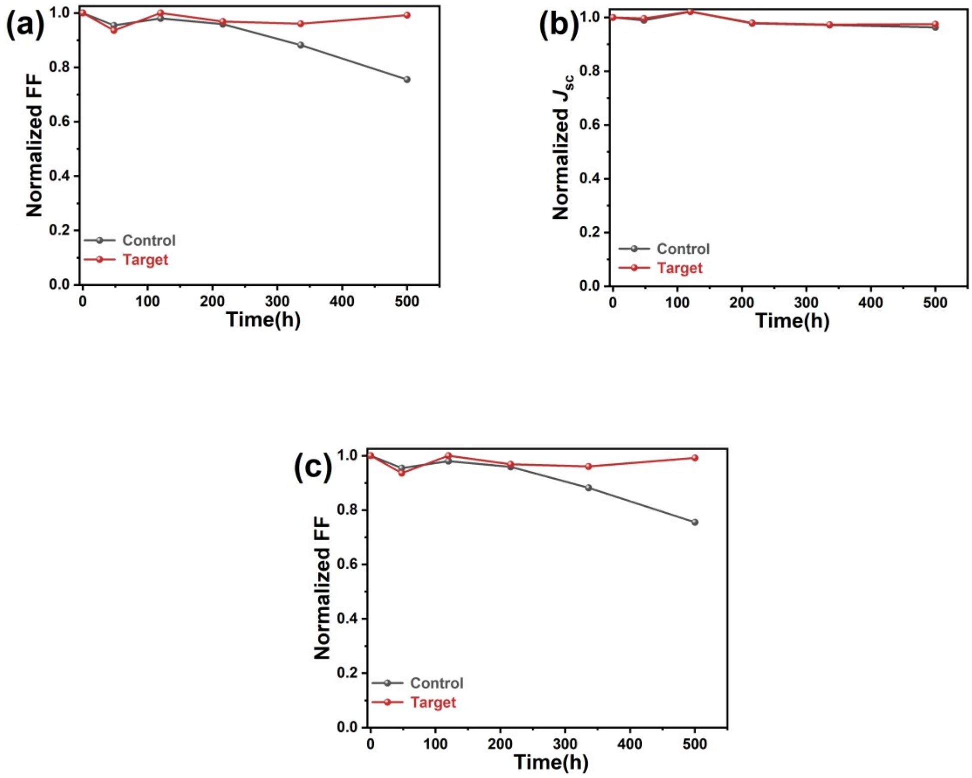

Figure S7. (a-c) The photovoltaic parameters degradation of control and Rutin-treated PSCs as a function of storage time under 85 ℃.

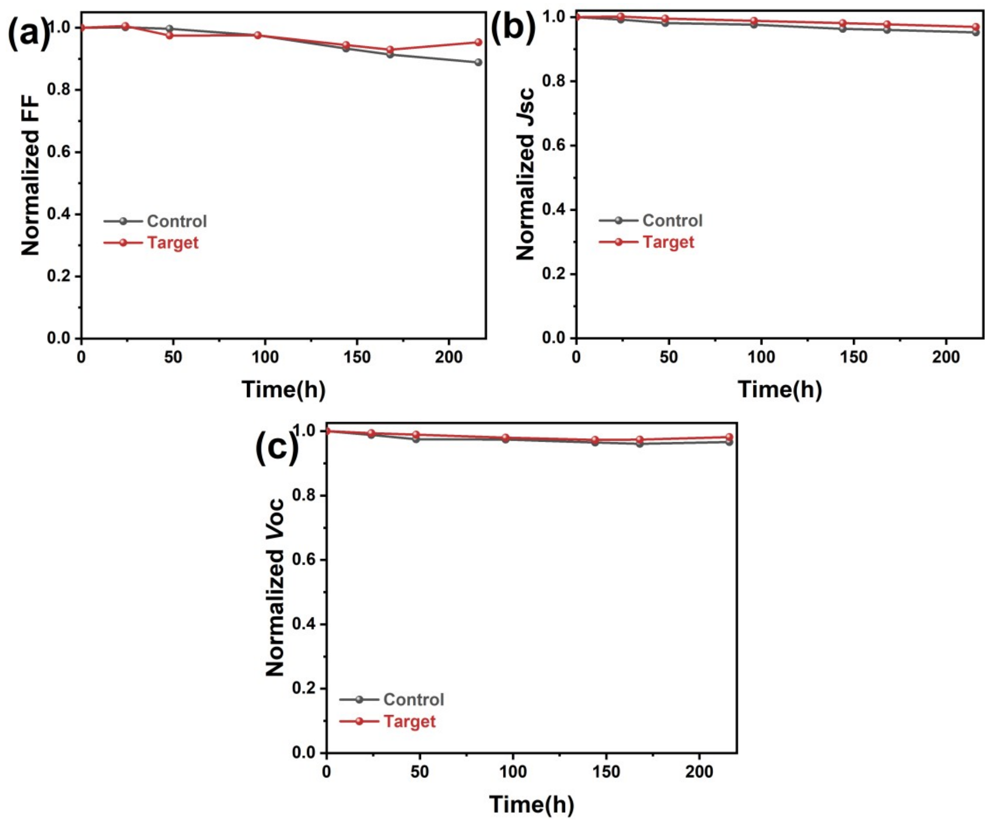

Figure S8. (a-c) The photovoltaic parameters degradation of control and Rutin-treated PSCs as a function of storage time under 25 ℃, 10% RH.

Table S1. Summary of the photovoltaic data for previously reported $CsPbI_2Br$ (carbon electrode).

Based on $CsPbI_2Br$ (carbon electrode)					
Device architecture	J_{SC} (mA cm^{-2})	V_{OC} (V)	FF (%)	PCE (%)	Ref.
FTO/c-TiO_2/$CsPbI_2Br$/Carbon	**14.84**	**1.320**	**77.1**	**15.10**	**This work**
FTO/c-TiO_2/$CsPbI_2Br$/Carbon	14.18	1.21	75.90	13.08	1
FTO/TiO_2/$CsPbI_2Br$/Carbon	15.70	1.312	74.00	15.24	2
FTO/TiO_2/$CsPbI_2Br$/NPTMS/Carbon	14.78	1.13	61.00	10.22	3
FTO/c-TiO_2/$CsPbI_2Br$/Carbon	13.30	1.14	73.86	11.24	4
ITO/c-TiO_2/$CsPbI_2Br$/ATHPBr/Carbon	14.28	1.30	78.11	14.50	5
ITO/SnO_2/$SnCl_2$/$CsPbI_2Br$/Carbon	14.74	1.26	74.00	13.78	6
ITO/SnO_2/$CsPbI_2Br$/BrAL/Carbon	13.68	1.21	68.80	11.34	7
FTO/TiO_2/$CsPbI_2Br$/Carbon	14.60	1.19	73.60	12.78	8
FTO/TiO_2/PVP-$CsPbI_2Br$/Spiro-OMeTAD/Carbon	18.47	1.01	56.35	10.47	9
FTO/SnO_2/$CsPbI_2Br$/Carbon	14.51	1.30	71.02	13.38	10
FTO/TiO_2/$BMIMBF_6$/$CsPbI_2Br$/Carbon	14.33	1.22	75.27	13.19	11
ITO/SnO_2/$CsPbI_2Br$/$BMIMBF_4$/Carbon	14.68	1.27	75.00	14.03	12
FTO/TiO_2/MABr-$CsPbI_2Br$/Carbon	16.62	1.21	74.00	14.84	13
FTO/TiO_2/$CsPbI_2Br$/CuPc/Carbon	14.33	1.22	75.00	13.16	14
ITO/SnO_2/$SnCl_2$/$CsPbI_2Br$/Cs_2PtI_6/Carbon	14.85	1.28	72.00	13.69	15
FTO/c-TiO_2/m-TiO_2/$CsPbI_2Br$/Carbon black/Carbon	14.94	1.21	72.59	13.13	16
ITO/SnO_2/$CsPbI_2Br$/SnPc/Carbon	13.69	1.24	66.90	11.39	17
FTO/TiO_2 NRAs/$CsPbI_2Br$/Carbon	14.39	1.15	69.10	11.45	18
FTO/TiO_2/$CsPbI_2Br$/Carbon	14.47	1.25	80.10	14.49	19
FTO/c-TiO_2/m-TiO_2/Al_2O_3/Mg-$CsPbI_2Br$/NiO/Carbon	14.75	1.06	69.00	10.80	20
FTO/c-TiO_2/m-TiO_2/La-$CsPbI_2Br$/Carbon	11.66	1.12	61.24	8.03	21
FTO/SnO_2/$CsPbI_{2+x}Br_{1-x}$/Carbon	15.46	1.23	64.00	12.19	22

ITO/SnO_2/KOH/$CsPbI_2Br$/Carbon	13.89	1.21	68.71	11.78	23
ITO/SnO_2/$CsPbI_2Br$/Co_3O_4/Carbon	13.09	1.19	72.12	11.21	24
ITO/SnO_2/$CsPbI_2Br$/PMMA/Carbon	12.64	1.202	71.00	10.95	25
ITO/SnO_2/$CsPbI_2Br$/CuPc/Carbon	13.61	1.22	66.30	11.04	26
ITO/SnO_2/$CsPbI_2Br$/Carbon	14.25	1.14	64.12	10.44	27
FTO/SnO_2/$CsPbI_2Br$/Carbon	14.29	1.33	70.96	13.52	28
ITO/SnO_2/Nb-$CsPbI_2Br$/Carbon	12.06	1.20	72.00	10.42	29
FTO/TiO_2/$CsPbI_2Br$/P3HT-MWCNT/Carbon	13.35	1.21	62.00	10.01	30
FTO/c-TiO_2/m-TiO_2/Al_2O_3/$CsPbI_2Br$/NiO/Carbon	14.33	0.94	62.50	8.44	31
FTO/TiO_2/$CsPbI_2Br$-HTAB/Carbon	14.10	1.26	80.60	14.30	32
ITO/SnO_2/$CsPbI_2Br$/Carbon	12.91	1.19	66.10	10.13	33
FTO/c-TiO_2/$CsPbI_2Br$/Carbon	13.87	1.15	64.00	10.21	34
FTO/c-TiO_2/$CsPbI_2Br$/Carbon	13.54	1.15	64.20	10.00	35
FTO/Nb_2O_5/$Cs_{0.99}Rb_{0.01}PbI_2Br$/Carbon	14.02	1.24	69.00	12.00	36
FTO/c-TiO_2/$CsPbI_2Br$/P-QD/Carbon	14.52	1.309	79.11	15.04	37
FTO/SnO_2-Cl/$CsPbI_2Br$-Cl/Carbon	14.70	1.26	76.17	14.11	38
FTO/TiO_2/$CsPbI_2Br$/Carbon	14.28	1.324	80.73	15.27	39
ITO/SnO_2/KTFA/$CsPbI_2Br$/CF_3PMABr/Carbon	14.98	1.273	73.7	14.05	40
ITO/SnO_2/MAAc-$CsPbI_2Br$/Carbon	14.20	1.27	61.80	11.20	41
ITO/c-TiO_2/$CsPbI_2Br$/Carbon	14.21	1.28	79.40	14.46	42
ITO/SnO_2/$SnCl_2$/$CsPbI_2Br$/PTU/Carbon	14.83	1.22	72.00	13.01	43
ITO/SnO_2/ZnO/E-K/$CsPbI_2Br$/Carbon	14.95	1.255	74.30	13.94	44
FTO/SnO_2/$CsPbI_2Br$+3Br-PABr/Carbon	14.60	1.28	75.14	14.04	45
ITO/SnO_2/ZnO-EAD/$CsPbI_2Br$/Carbon	14.98	1.272	76.50	14.58	46
FTO/c-TiO_2/m-TiO_2/$CsPb_2I_4Br$-$CsPbI_2Br$ BHJ/Carbon	14.60	1.32	79.11	15.25	47
ITO/SnO_2/ZnO/$CsPbI_2Br$/P-F-PEABr/Carbon	14.91	1.269	73.80	13.97	48
FTO/TiO_2@Sb_2S_3-MPA/$CsPbI_2Br$/Carbon	14.50	1.29	77.49	14.59	49
FTO/SnO_2/$CsPbI_2Br$/Fe_3O_4@NC UVO/Carbon	15.31	1.26	64.00	12.25	50
FTO/SnO_2/$Pb(Ac)_2$-$CsPbI_2Br$/Carbon	15.87	1.32	65.00	13.73	51
FTO/TiO_2/$CsPbI_2Br$/CNT/P3HT/Carbon	14.63	1.355	78.50	15.56	52
FTO/SnO_2/AA-$CsPbI_2Br$/Carbon	14.50	1.22	72.00	12.71	53

FTO/TiO_2/NaSCN-$CsPbI_2Br$/Carbon	14.31	1.267	80.70	14.63	54
FTO/SnO_2/$CdCl_2$/$CsPbI_2Br$/Carbon	14.30	1.30	77.85	14.47	55
FTO/TiO_2+MXene/$CsPbI_2Br$/Carbon	14.961	1.289	80.26	15.48	56
FTO/TiO_2/$CsPbI_2Br$/EAI+PEAI/Carbon	14.59	1.17	80.32	13.76	57
FTO/TiO_2/$CsPbI_2Br$/CSI/Carbon	14.51	1.267	79.81	14.67	58
FTO/c-TiO_2/$CsPbI_2Br$/NiOx/NiOx@Carbon	14.82	1.31	77.31	15.01	59
FTO/c-TiO_2/$CsPbI_2Br$-MWCNT/Carbon	14.85	1.291	79.00	15.14	60
ITO/SnO_2/$CsPbI_2Br$/1-B-3-$MTMPF_6$/Carbon	14.69	1.200	76.00	13.47	61
FTO/TiO_2/ET/$CsPbI_2Br$/Carbon	14.14	1.308	78.71	14.56	62
FTO/TiO_2/PFPA/$CsPbI_2Br$/Carbon	14.79	1.21	79.07	14.15	63
ITO/SnO_2/$CsPbI_2Br$/BMIMMS/Carbon	15.13	1.23	71.2	13.25	64
FTO/SnO_2/$CsPbI_2Br$/DC/Carbon	15.96	1.26	70	14.08	65
FTO/TiO_2-BAP/$CsPbI_2Br$/PCBM/Carbon	14.88	1.27	78.99	14.9	66
FTO/TiO_2/$CsPbI_2Br$-PFPA/Carbon	14.8	1.21	79.07	14.15	67
FTO/TiO_2/$CsPbI_2Br$/(Sb_2S_3/PbS)/Carbon	14.93	1.28	77.11	14.73	68
FTO/TiO_2/$CsPbI_2Br$/(0D/3D)/Carbon	15.91	1.33	72	15.24	69
FTO/SnO_2/$CsPbI_2Br$-Ln$(OTF)_3$/Tm$(OTF)_3$/Carbon	14.96	1.312	77.1	15.13	70
FTO/SnO_2/$CsPbI_2Br$/F_3EACl/Carbon	14.6	1.28	78.62	14.69	71
FTO/SnO_2-PS/$CsPbI_2Br$/Carbon	14.12	1.25	74.5	13.11	72
FTO/c-TiO_2/$CsPbI_2Br$-TRP/Carbon	14.76	1.30	80.85	15.51	73
FTO/c-TiO_2/$CsPbI_2Br$ /Carbon	14.4	1.344	79.43	15.37	74
FTO/c-TiO_2/IMA/$CsPbI_2Br$-BTFBT/Carbon	14.576	1.322	78.59	15.12	75
FTO/c-TiO_2/$CsPbI_2Br$/(2D/3D)/Carbon	14.81	1.34	77	15.29	76

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