Supporting Information

One-dimensional (1D) [6, 6]-phenyl-C61-butyric acid methyl ester (PCBM) nanorods as efficient additive for improving the efficiency and stability of perovskite solar cells

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Experimental Section

Synthesis of 1D PCBM nanorods

1D PCBM nanorods were synthesized according to the previously reported procedure of liquid-liquid interfacial precipitation (LLIP).[S1] Briefly, PCBM (Nano-C) was dissolved in chloroform with a concentration of 1 mg/mL and ultrasonicated for 30 min to produce a homogeneous dispersion. The PCBM chloroform solution was then heated up to 60 °C and methanol was gently added at a volume ratio of 10 mL methanol to 1 mL PCBM solution. Thereafter, the mixture solution was sonicated for 5 min (FS30 ultrasonic cleaner, Fisher Scientific) and stored at room temperature for 24 h. Finally, the 1D PCBM nanorods were participated out after another 30 min sonication, centrifuged and dried under vacuum, and redispersed in DMF at a concentration of 1 or 5 mg/mL for subsequent use.

Synthesis of methylammonium iodide (MAI)

CH_3NH_3I was synthesized according to reported procedures.[S2] In a typical experiment, a hydroiodic acid (30 mL, 0.227 mol, 57 wt.% in water, Aldrich) and methylamine (27.8 mL, 0.273 mol, 40% in ethanol, Aldrich) were mixed and stirred in a 250 mL round bottom flask in an ice bath for 2 h. After stirring at 0 °C for 2 h, the resulting solution was recovered by rotary evaporation at 80 °C for 1 h to produce MAI. The product was washed three times with diethyl ether, and then was dissolved in ethanol, recrystallized from diethyl ether, and dried at 60 °C in a vacuum oven for 24 h.

Characterization

Scanning electron microscope (SEM) images were recorded on a JSM-7000F field emission scanning electron microscope (FESEM, Japan Electron Optics Labortary Co., Ltd., JEOL). Transmission electron microscopy (TEM) and high-resolution TEM (HRTEM) images were obtained with a JEM-2100 transmission electron microscope (Japan Electron Optics Laboratory Co., Ltd., JEOL) with an accelerating voltage of 200 kV. X-ray diffraction (XRD) was carried out using Miniflex II Desktop X-ray Diffractometer. UV–vis absorption was measured with a Shimadzu UV1800 spectrometer. PL spectroscopic measurements were performed on a Gilden Photonics PL spectrophotometer.

Device fabrication

The perovskite solar cells were fabricated by a simple one-step deposition-crystallization method reported previously with some modification.[S3] ITO glass substrates were cleaned sequentially with detergent, deionized water, acetone, and isopropyl alcohol, followed by drying with N_2 flow and UV–ozone treatment for 20 min. The PEDOT:PSS solution (Al4083 from H. C. Starck) was spin-cast onto ITO electrodes at 5000 rpm for 60 s, followed by heating at 150 °C for 10 min. The PEDOT: PSS-coated ITO/Glass was then transferred to an Ar-filled glove box. To a mixture of 115 mg of PbI_2 and 40 mg of CH_3NH_3I in DMF, 1D PCBM nanorods were gradually added to form 1.2 M $CH_3NH_3PbI_3$ (0.208 mL) solutions, with the 1D PCBM nanorod concentration from 0 to 960 μg/mL. Then, 40 μL each of the resultant solutions was spin-coated onto the ITO/Glass pre-coated with PEDOT: PSS at 800 rpm for 10 s, followed by 4000 rpm for 20s while 150 μL chlorobenzene was quickly

dropped on the substrate. The perovskite-coated film was then annealed on a hot plate at 110 °C for about 15 min. Finally, the resultant device was transferred to the evaporator for thermal evaporation of Ca (20 nm) and Al (100 nm) at a pressure of 10^{-7} Torr. The active area of each device is 0.12 cm^2, as defined by the overlap of the ITO and the thermally evaporated Al.

Device Characterization

All the devices were tested in an Ar-filled glovebox using a Keithley 2400 source meter and a Newport Oriel sol 2A solar simulator (300 W). The light intensity was calibrated to be 100 mW cm^{-2} using a calibrated Si solar cell and a KG5 color filter. The device performance parameters were obtained from the J–V curves of the solar cells under illumination. The incident photon-to-current efficiency (IPCE) was measured on a Solar Cell Measurement System from PV measurement Inc. We used the 91150V Reference Cell and Meter (ORIEL instrument) to calibrate the light intensity prior to the device testing.

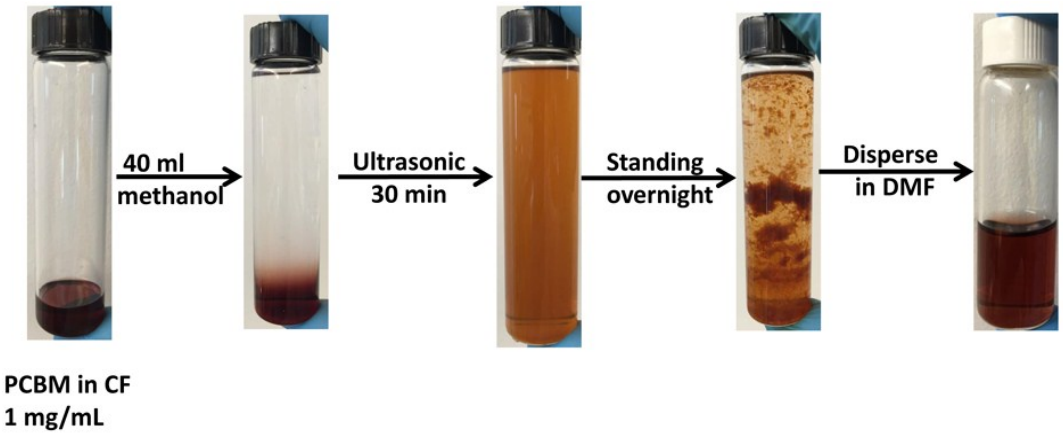

Fig. S1. Synthesis procedure of 1D PCBM nanorods (see text).[S1]

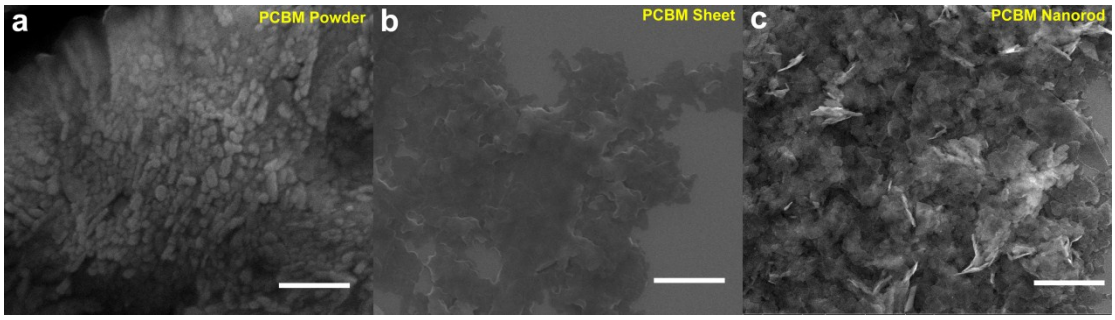

Fig. S2. The low magnification SEM images of (a) pristine PCBM powder, (b) PCBM sheet and (c) PCBM nanorod. Scale bar: 1 μm.

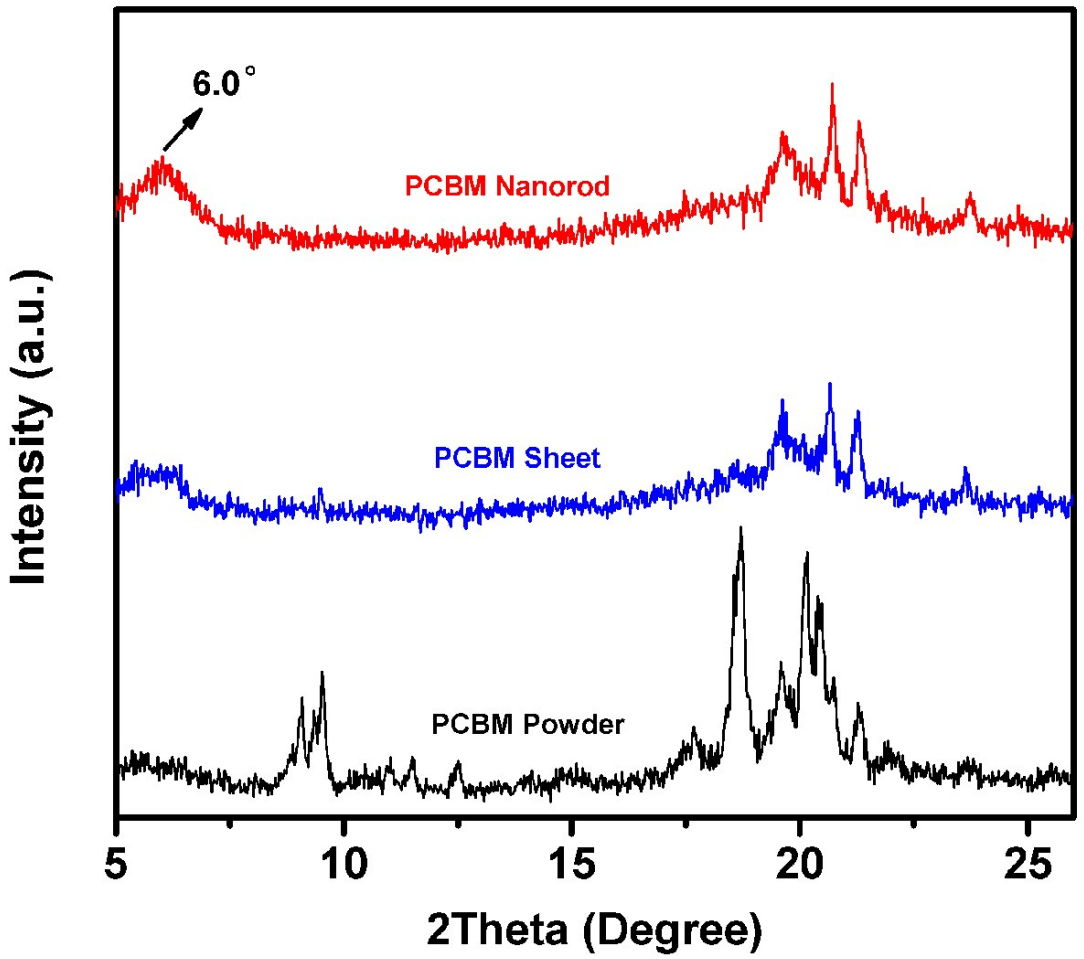

Fig. S3 XRD patterns for PCBM powder (black), PCBM sheets (blue) and PCBM nanorods (red).

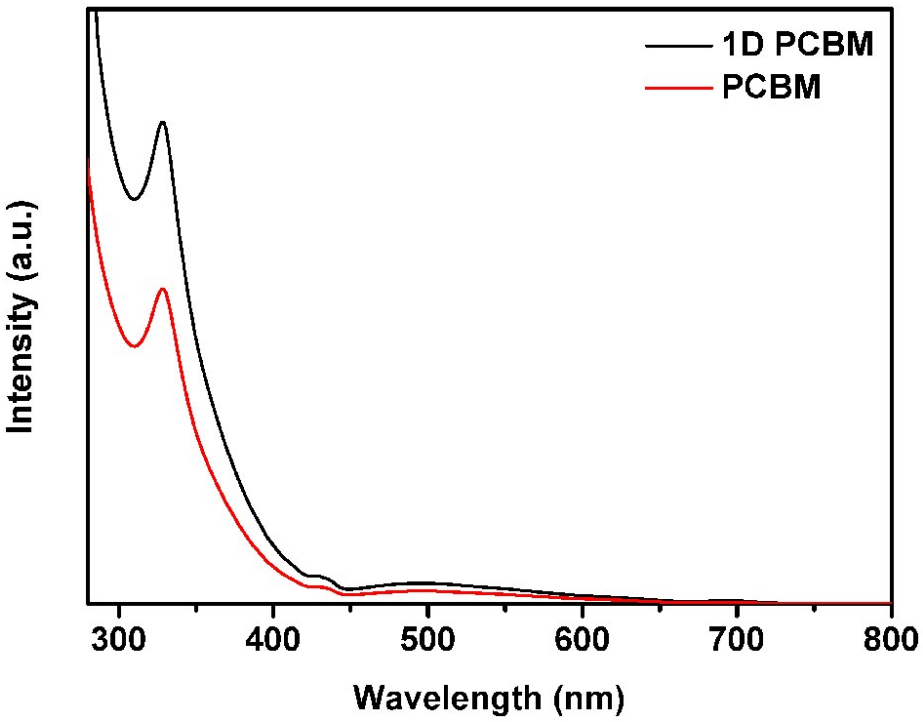

Fig. S4. UV-Vis spectrum of 1D PCBM nanorods and pristine PCBM in DMF solution.

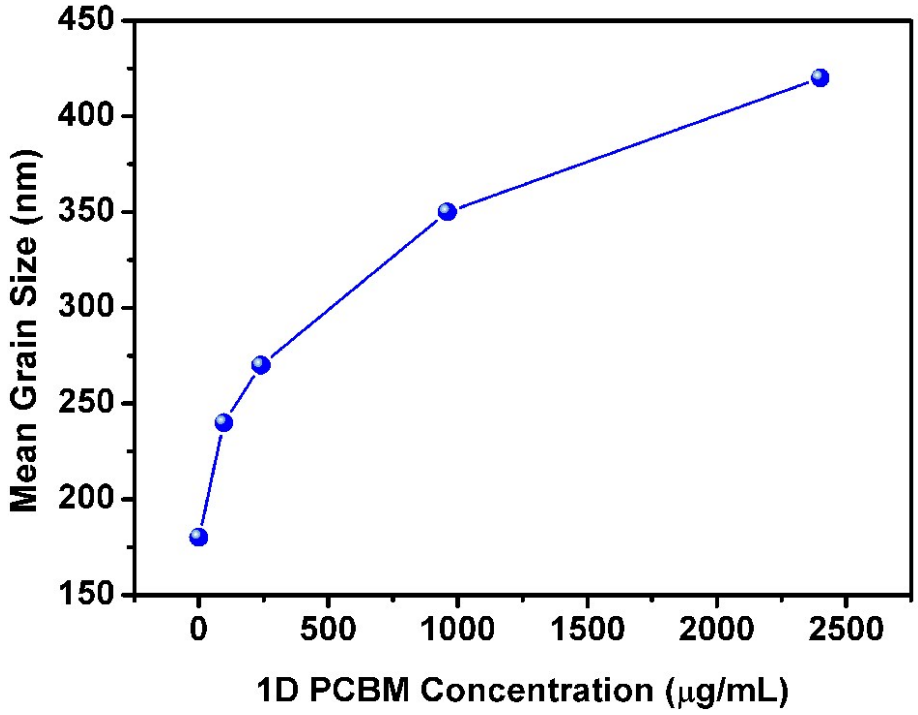

Fig. S5. The change in mean grain size of the perovskite film in the function of the concentration of 1D PCBM nanorods in PbI_2/MAI precursor solution.

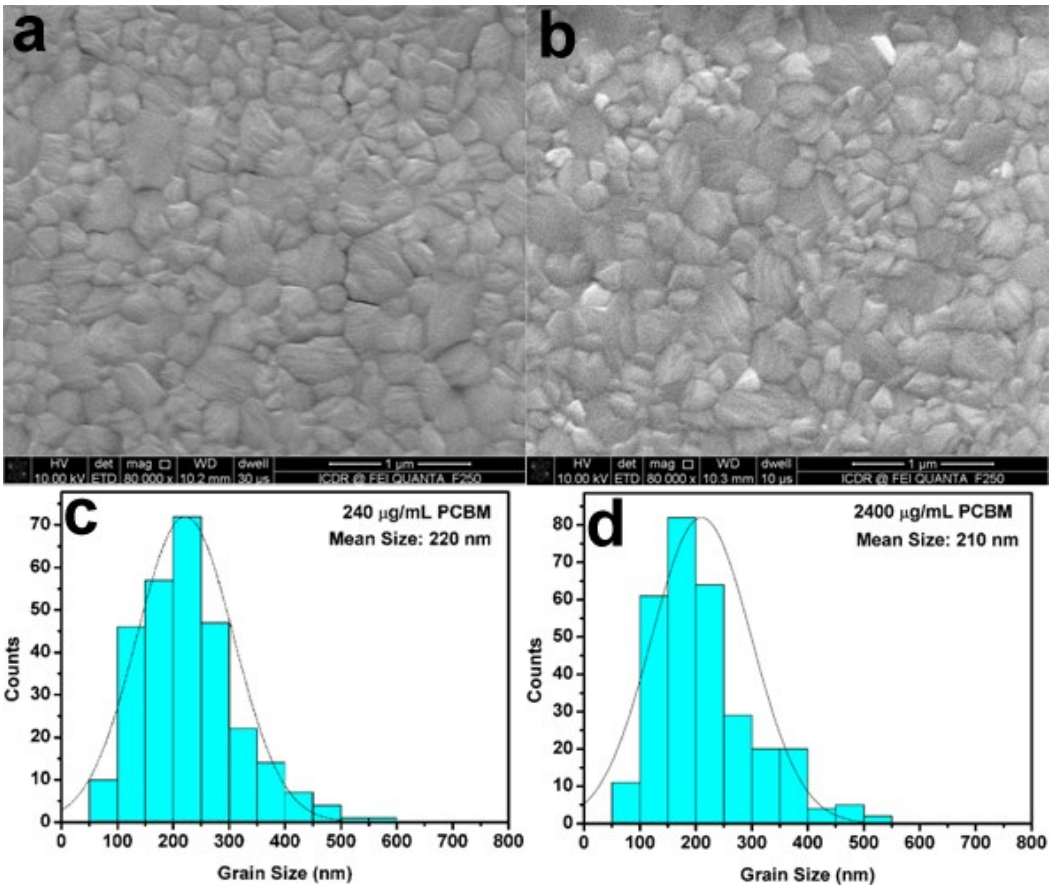

Fig. S6. SEM images of perovskite films with different content of pristine PCBM powder as additives under different magnification: (a) 240 μg/mL and (b) 2400 μg/mL. (c, d) show the corresponding histograms of grain size distribution.

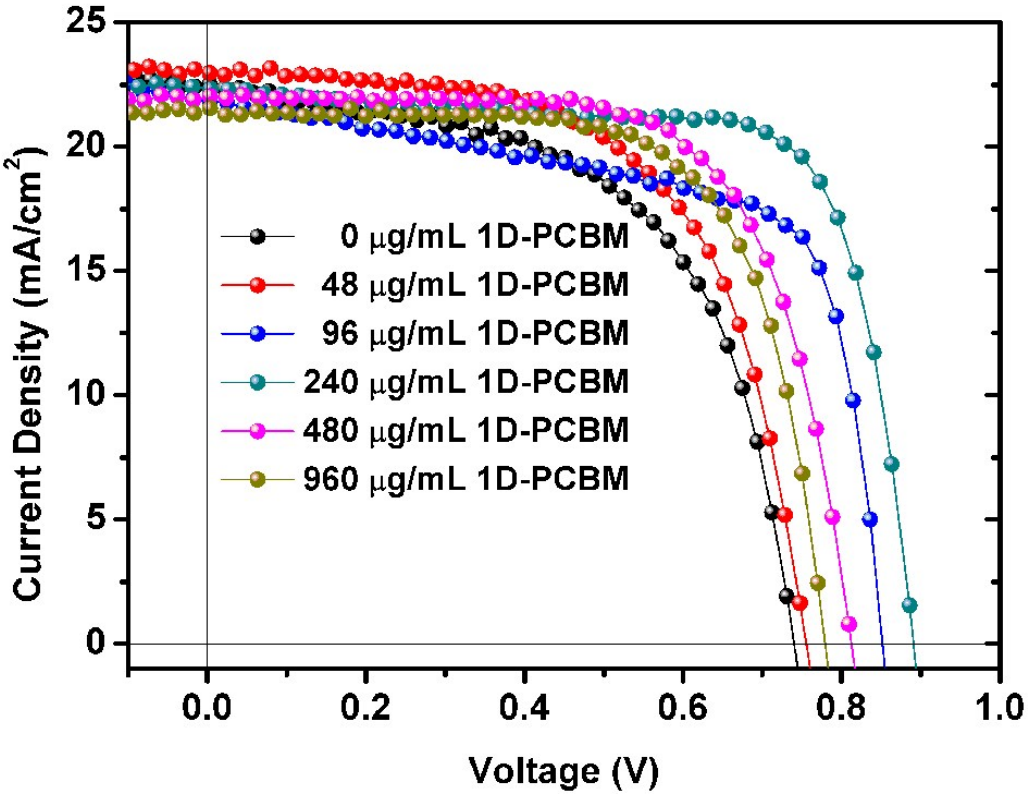

Fig. S7. J–V characteristics of the $CH_3NH_3PbI_3$ perovskite solar cells with different concentrations of the 1D PCBM nanorods.

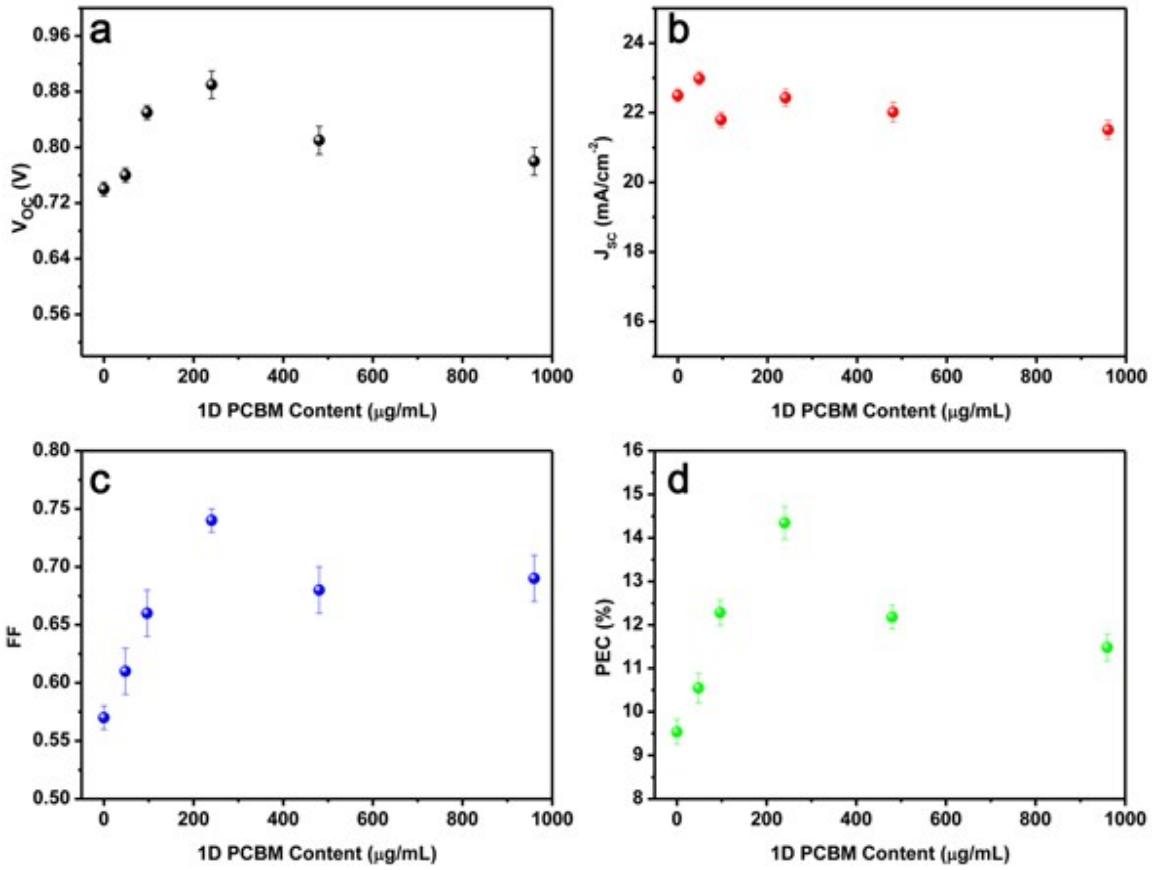

Fig. S8. (a)V_{OC}, (b) J_{SC}, (c) FF and (d) PCE of the PSCs under increasing dosage of 1D PCBM in perovskite layer.

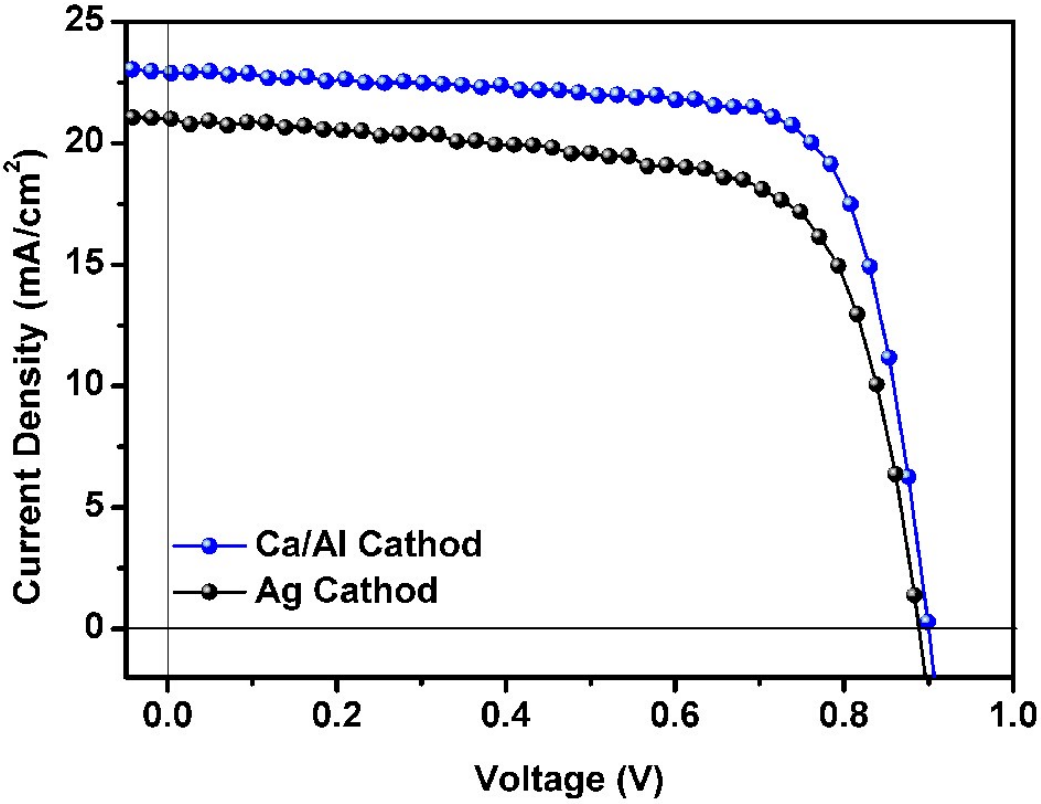

Fig. S9. The J-V curves of the devices using different cathods.

Table S1. Detailed parameter of the grain size data of the perovskite film obtained from SEM image.

Additive	Concentration (μg/mL)	Max. Grain Size (nm)	Min. Grain Size (nm)	Mean Grain Size (nm)
1D PCBM	0	510	40	180
1D PCBM	96	500	70	240
1D PCBM	240	590	80	270
1D PCBM	960	780	110	350
1D PCBM	2400	800	110	420
PCBM powder	240	570	50	220
PCBM powder	2400	530	70	210

Reference

S1 E. Gracia-Espino, H. R. Barzegar, T. Sharifi, A. M. Yan, A. Zettl and T. Wagberg, *ACS Nano*, 2015, **9,** 10516.

S2 Y. H. Chen, T. Chen and L. M. Dai, *Adv. Mater.*, 2015, **27**, 1053.

S3 M. D. Xiao, F. Z. Huang, W. C. Huang, Y. Dkhissi, Y. Zhu, J. Etheridge, A. Gray-Weale, U. Bach, Y. B. Cheng and L. Spiccia, *Angew. Chem. Int. Edit.*, 2014, **53,** 9898.