

Drop-coating produces efficient CsPbI₂Br solar cells

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SUPPORTING INFORMATION

Experimental section

Materials

All materials were purchased and used without further purification unless specified. Dimethyl formamide (DMF) (99.8%), dimethyl sulfoxide (DMSO) (99.9%), chlorobenzene (99.8%), and CsI (99.999%) were purchased from Alfa Aesar. PbI₂ (98.0%) was purchased from TCI. PbBr₂ (99.999%) was purchased from Sigma Aldrich. Isopropanol (IPA) (99.5%) was purchased from J&K. The SnO₂ (tin (IV) oxide colloidal dispersion, 15% in H₂O) was purchased from Alfa Aesar. Poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine] (PTAA, Mn = 6000–15 000) was purchased from Xi'an Polymer Light Technology Corp.

Precursor preparation

SnO₂ colloidal dispersion was diluted with DI water in a weight ratio of 1 : 5 for the preparation of SnO₂ layer. 0.6 M CsPbI₂Br solution was made by mixing 1.2 mmol CsI, 0.6 mmol PbI₂, and 0.6 mmol PbBr₂ in 1 mL DMSO/DMF (v/v, 1 : 4) mixed solvent. 50 μL of IPA was added into 1 mL CsPbI₂Br solution to improve the wettability. ZnO and D-PTAA solution were prepared according to our previous paper^[1]. PC₆₁BM solution was prepared by dissolved 20 mg PC₆₁BM in 1 mL chlorobenzene.

Device fabrication

Patterned ITO glass with a sheet resistance of 15 Ω sq⁻¹ was cleaned by ultrasonics in detergent, deionized water, acetone, isopropanol sequentially and then treated with UV-ozone for 10 min. SnO₂ colloidal dispersion was spin-coated onto ITO glass at 3000 rpm for 30 s and annealed at 150 °C in air for 30 min. ZnO precursor solution was spin-coated onto SnO₂ layers at 4000 rpm for 30 s and annealed at 200 °C in air for 20 min. Then the substrates were treated with UV-ozone for 4 min. CsPbI₂Br films were made by drop-coating or spin-coating. For the drop-coating, the substrates were placed on a 65 °C hot-plate, after 1 min 1 μL of CsPbI₂Br precursor solution was deposited onto the center of a substrate. Then the solution can spread on the substrate spontaneously and form a round film in a few seconds. A stream of nitrogen applied

to the film to accelerate the drying process, resulting in a brown film. Then the films were annealed at 250 °C in N₂ box for 10 min. For the spin coating, 1 M CsPbI₂Br precursor solution was spin-coated onto the substrate at 3000 rpm for 30 s, then the films were annealed at 250 °C for 10 min. The whole spin-coating process is conducted in glove-box. After cooling to room temperature, D-PTAA was spin-coated onto CsPbI₂Br according to our previous paper. Finally, MoO₃ (~6 nm) and Ag (~80 nm) were evaporated onto D-PTAA through a shadow mask under vacuum (ca. 10⁻⁵ Pa). The effective area for the devices is 4 mm². For the electron-only device, PC₆₁BM was used instead of the D-PTAA/MoO₃. PC₆₁BM layer was prepared by spin coating PC₆₁BM solution at 1500 rpm for 25 s.

Characterizations

J-*V* curves were measured by using a computerized Keithley 2400 SourceMeter and a Xenon-lamp-based solar simulator (Enli Tech, AM 1.5G, 100 mW/cm²). External quantum efficiency (EQE) was measured by using a QE-R3011 measurement system (Enli Tech). Absorption spectra were recorded on a Shimadzu UV-1800 spectrophotometer. Top-view scanning electron microscopy (SEM) image was performed on a Hitachi SU-8200 field emission SEM. Cross-sectional SEM image was performed on a JC-Zeiss Merlin field emission SEM. Atomic force microscopy (AFM) image was performed on Bruker Multimode-8 scanning probe microscope. The steady-state photoluminescence (PL) and time-resolved PL was performed on FLS1000 spectrometer.

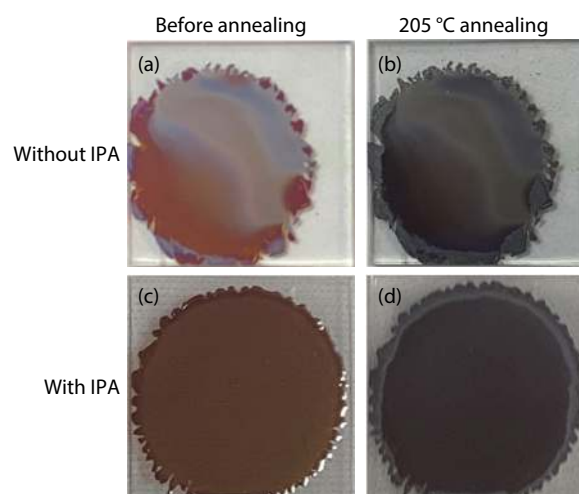


Fig. S1. (Color online) Photographs for CsPbI₂Br films made without IPA or with 5% IPA (vol%).

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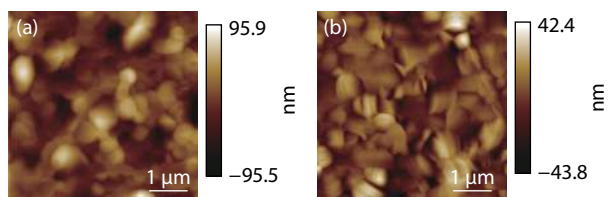


Fig. S2. (Color online) AFM height images for CsPbI₂Br films made (a) without IPA or (b) with 5% IPA.

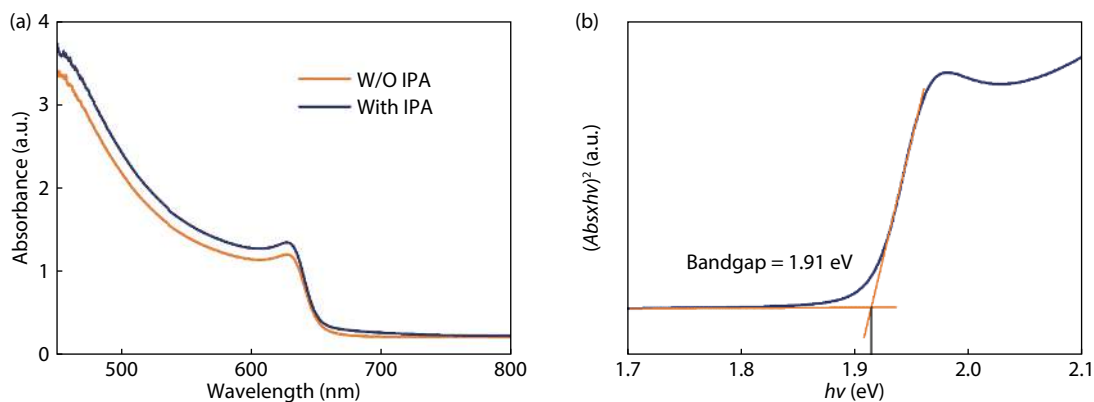


Fig. S3. (Color online) (a) Absorption spectra for CsPbI₂Br films made without IPA or with 5% IPA. (b) Tauc plot for the film made with 5% IPA.

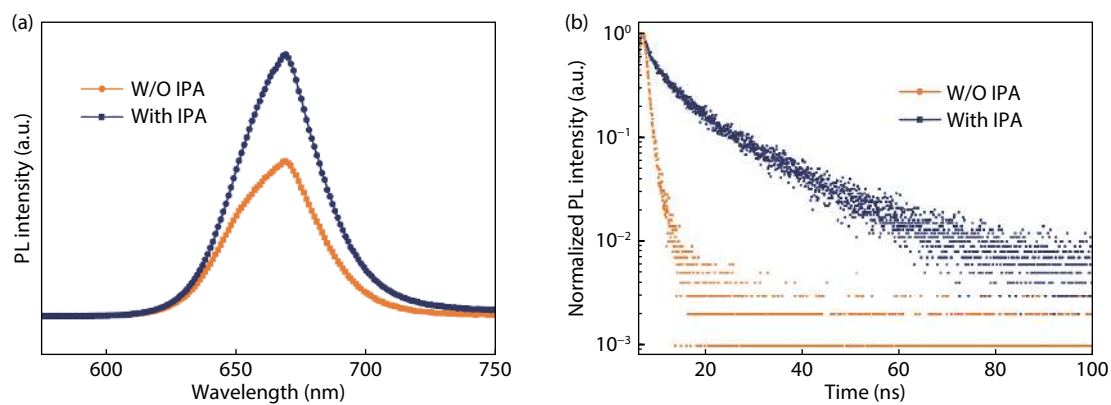


Fig. S4. (Color online) (a) Steady-state PL spectra. (b) Time-resolved PL spectra for CsPbI₂Br films made without IPA or with 5% IPA.

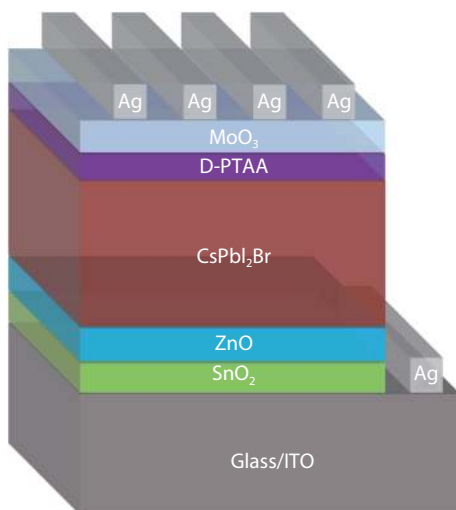


Fig. S5. (Color online) Structure for CsPbI₂Br solar cell.

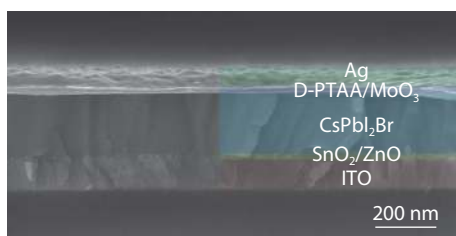


Fig. S6. (Color online) Cross-section SEM image for CsPbI₂Br solar cell.

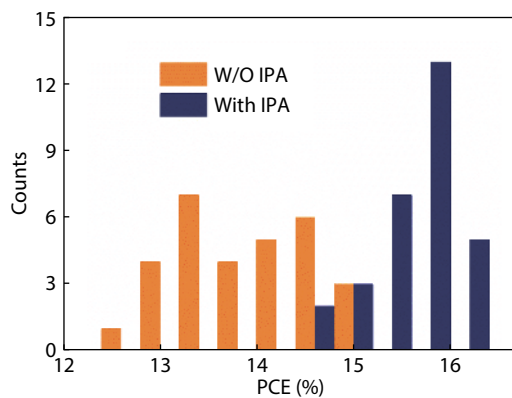


Fig. S7. (Color online) Histograms of PCEs for CsPbI₂Br solar cells made without or with 5% IPA.

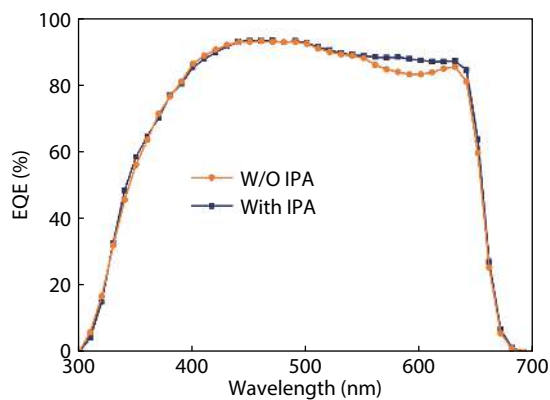


Fig. S8. EQE spectra for CsPbI₂Br solar cells made without or with 5% IPA.

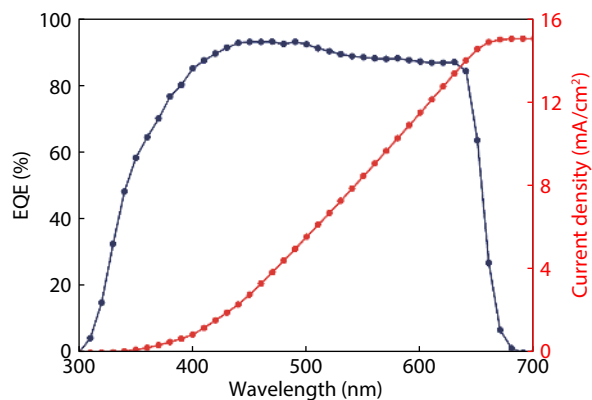


Fig. S9. EQE spectrum for the best cell.

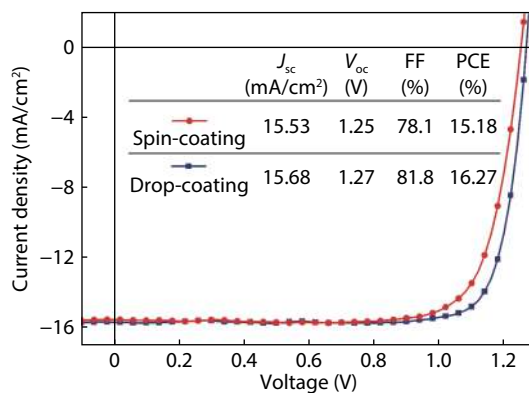
Fig. S10. J - V curves for PSCs made by spin-coating or drop-coating.

Table S1. FWHM of XRD peaks in Fig. 1(e).

	(100) peak	(200) peak
Without IPA	0.129°	0.199°
With IPA	0.119°	0.153°

Table S2. Intensity ratio of XRD peaks in Fig. 1(e).

	(100)/(110)	(200)/(110)
Without IPA	4.5	7.9
With IPA	23.3	43.0

Table S3. Optimization of IPA content in CsPbI₂Br precursor solution.

IPA content (vol%)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE ^a (%)
0	1.25	15.22	79.3	15.15 (13.92)
3	1.26	15.64	81.5	16.04 (15.46)
5	1.27	15.68	81.8	16.27 (15.57)
7	1.26	15.69	79.9	15.78 (15.40)

^aData in parentheses stand for the average PCEs for 30 devices.

Table S4. Optimization of substrate temperature.

Temperature (°C)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE ^a (%)
55	1.25	15.67	80.2	15.77 (15.25)
65	1.27	15.70	81.8	16.27 (15.57)
75	1.25	15.73	79.6	15.65 (14.98)

^aData in parentheses stand for the average PCEs for 30 devices.

Table S5. Performance of CsPbI₂Br solar cells made by drop-coating or spin-coating.

Method	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE ^a (%)
Drop-coating	1.27	15.68	81.8	16.27 (15.57)
Spin-coating	1.25	15.54	78.1	15.18 (14.52)

^aData in parentheses stand for the average PCEs for 30 devices.

References

- [1] Fang Z, Meng X, Zuo C, et al. Interface engineering gifts CsPbI_{2.25}Br_{0.75} solar cells high performance. *Sci Bull*, 2019, 64, 1743