

Supporting Information

Quasi Quantum Dots-Induced Stabilization of α -CsPbI₃ Perovskite for High-Efficiency Solar Cells

Cheng Liu,[‡] Yi Yang,[‡] Xin Liu, Yong Ding, Zulqarnain Arain, Xinye Li, Yuanlong Li, Zian Zhou, Songyuan Dai* and Mohammad Khaja Nazeeruddin**

Experimental Section

Solar cells fabrication: A compact TiO₂ layer was fabricated by spray method at 500°C as previous reported.¹ For the QQD CsPbI₃ film preparation, the CsPbI₃ precursor solution was prepared by dissolving 0.65 M of CsI (Alfa, 99.998%) and 0.65 M of PbI₂ (Alfa, 99.9985%) in DMF (Alfa, 99.8%). To improve the solubility of CsPbI₃, 33 μ L of hydroiodic acid (Aladdin, 57% w/w) was added to 1 mL of the precursor solution. 1-Adamantanemethylamine (ADMA, Acros, 98%) was then added with a typical ratio of 7 mM (0.25wt%) in the solution. The completely dissolved precursor solution was spin-coated onto the substrates at 2000 rpm for 30 s with ramps of 500 rpm·s⁻¹ in a nitrogen glovebox. The precursor film was then transferred onto a hotplate to be annealed at 100°C for 10 min. A spiro-OMeTAD/chlorobenzene solution (70 mM) with additives of 32 μ L of 4-tert-butylpyridine (TBP) and 20 μ L of Li-TFSI/acetonitrile (1.8 M) was spin-coated on top of the active layer at 5000 rpm for 30 s. Finally, an 80-nm-thick gold electrode was deposited by thermal evaporation.

Characterization: UV-vis spectra were recorded using a UV/Vis spectrometer (Shimadzu, UV-3600) in the 400 nm - 800 nm range. SEM images were measured with

a Hitachi SU8010 microscope to characterize the film morphology and device structures. XRD spectra of the inorganic perovskite films were recorded with a Rigaku SmartLab SE X-ray diffractometer. The J - V characteristics of the photovoltaic devices were measured with a Keithley 2420 sourcemeter under a simulated AM 1.5G spectrum and a solar simulator (XES-300T1, SAN-EI Electric), which was calibrated using a standard silicon reference cell. The J - V curves were all measured by masking the active area of 0.09 cm² with a scanning rate of 50 mV·s⁻¹ in the nitrogen atmosphere. The devices were measured both in reverse scan (2.1 V → -0.2 V, step 23 mV) and forward scan (-0.2 V → 2.1 V, step 23 mV). The devices were taken out for incident photon-to-current efficiency (IPCE) measurements, and IPCE was measured by an Enli Technology IPCE measurement system with a dual xenon/quartz halogen light source. Steady PL, TRPL and confocal PL mapping were recorded with a laser confocal Raman spectrometer (Princeton Instruments, Acton Standard Series SP-2558) and a 405 nm laser (OBIS LX-405) using a home-built confocal microscope on a 10 × 10 μm² sample area.

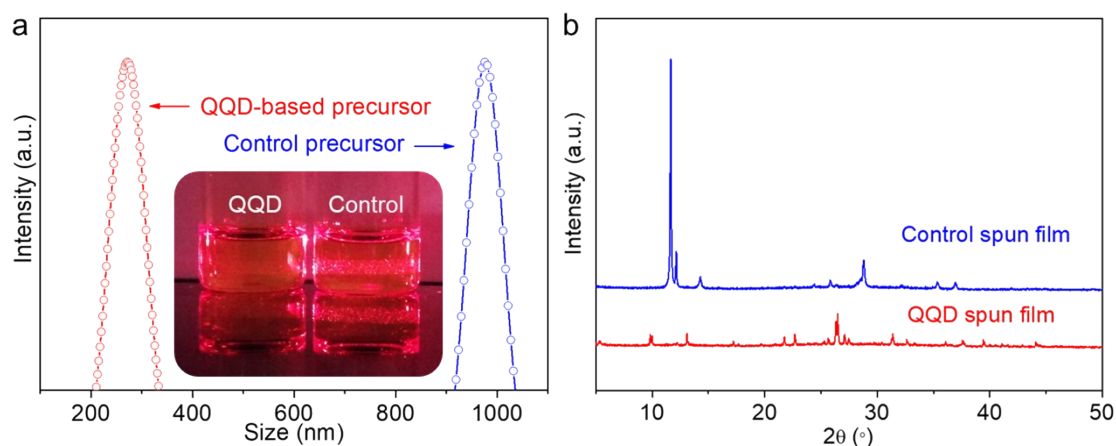


Fig. S1 a) Dynamic light scattering measurements on the CsPbI_3 -DMF solutions with ADMA ligands. Inset shown in a) is the image of Tyndall effect measurements for the CsPbI_3 precursor solution. b) XRD spectra of CsPbI_3 spun films prepared by precursor solutions.

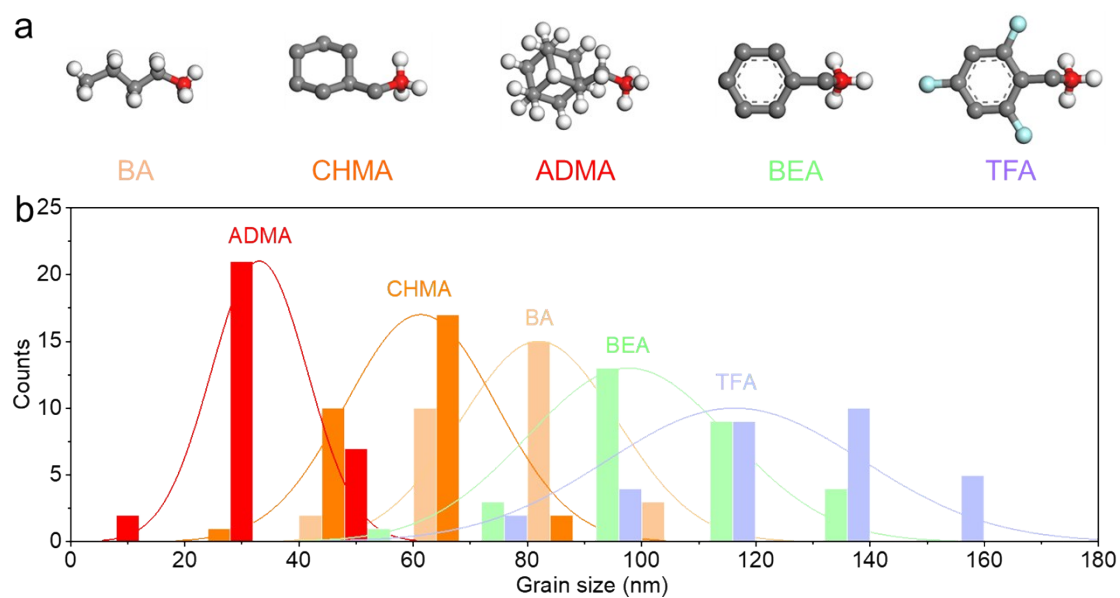


Fig. S2 (a) The geometry of Butylamine (BA), Cyclohexanemethylamine (CHMA), (Adamantan-1-yl)methan ammonium (ADMA), Benzylamine (BEA) and 2,4,6-Trifluorobenzylamine (TFA). (b) Cartogram of the grain sizes of the CsPbI_3 films using different ligands with the same concentration.

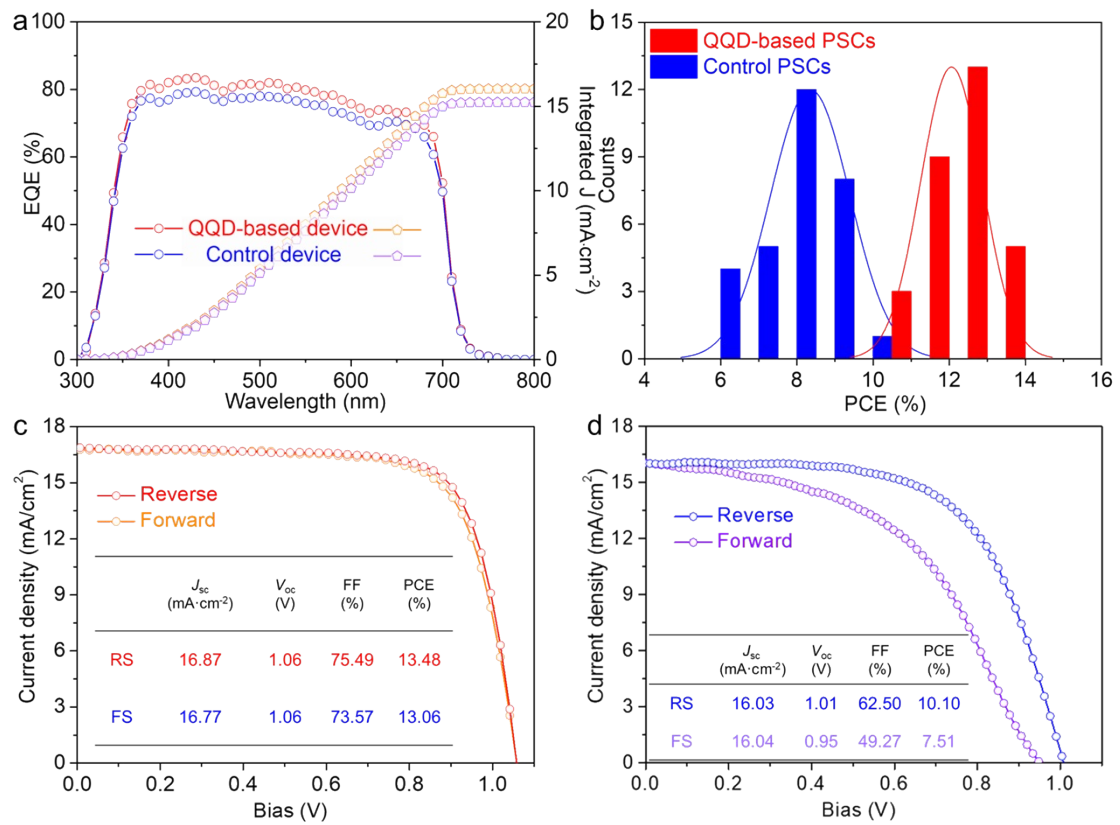


Fig. S3 a) EQE of the CsPbI₃ devices. b) Histograms of PCEs for 60 devices using the control and QD CsPbI₃ films. The $J-V$ curves with different scanning directions of c) the QD-based and d) the control device.

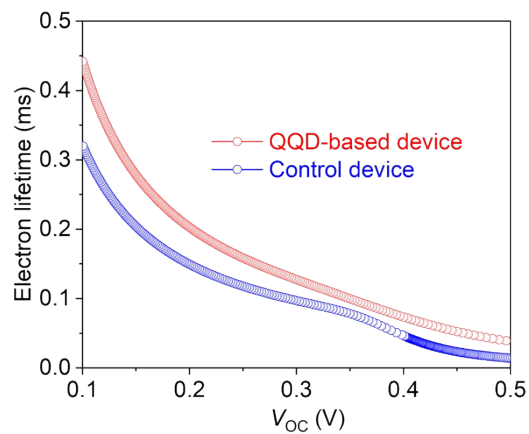


Fig. S4 The calculated electron lifetimes of the the QD-based and the control device.

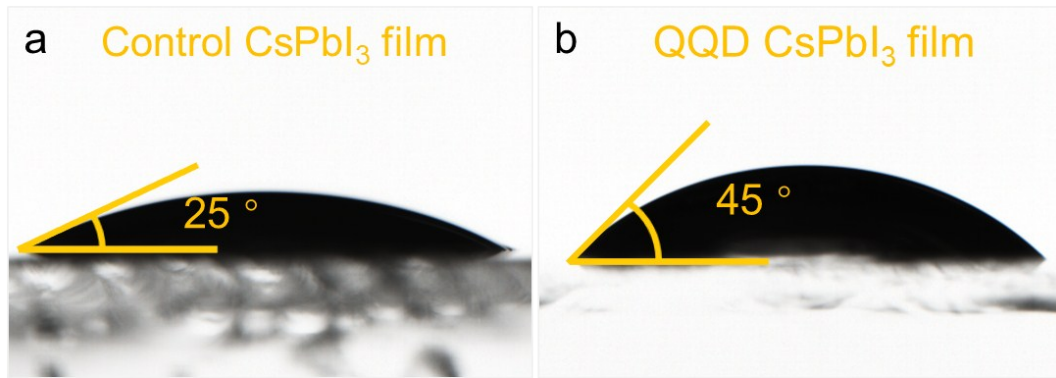


Fig. S5 The water contact angles on a) the control and b) QQD CsPbI₃ films.

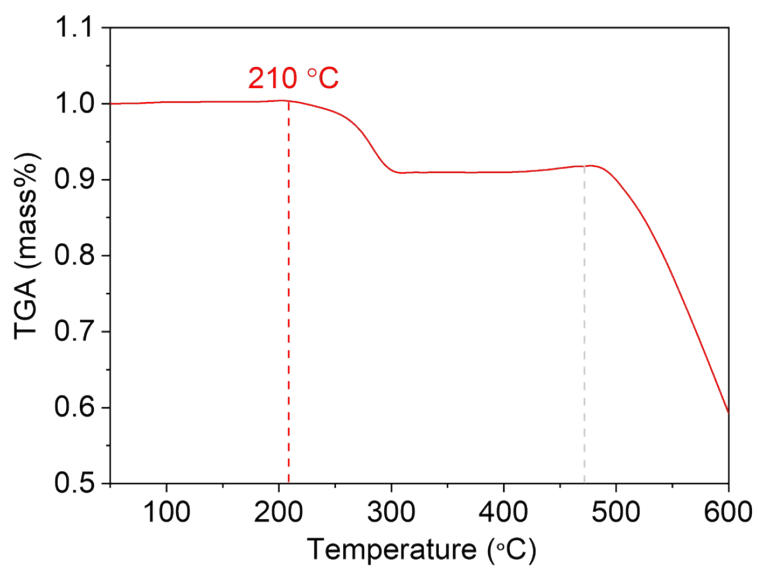


Fig. S6 Thermogravimetric analysis (TGA) curves of the QQD CsPbI₃ film.

Reference

- (1) Y. Yang, H. Peng, C. Liu, Z. Arain, Y. Ding, S. Ma, X. Liu, T. Hayat, A. Alsaedi and S. Dai, J. Mater. Chem. A, 2019, 7, 6450-6458.