Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Electronic Supplementary Material

Efficient and Stable Hybrid Conjugated Polymer/Perovskite Quantum Dot Solar Cell

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1.Materials

Cesium carbonate (Cs_2CO_3, 99.9%, Sigma), lead iodide (PbI_2, 99.9%, Adamas), 1-octandecene (ODE, 90%, J&k), oleic acid (OA, 90%, Aldrich), oleylamine (OAm, 90%, Aladdin), n-hexane (anhydrous 97.5%, J&K), n-octane (anhydrous, ≥ 98%, Alfa Aesar), methyl acetate (MeOAc, anhydrous 99%, J&k), toluene (analytical reagent, 98%, Chinasun Specialty Products Co., Ltd.), PFNBr titanium tetrachloride ($TiCl_4$, ≥98%, Sinopharm Chemical Reagent Co., Ltd.), tris(pentafluorophenyl)borane (95%, Acros Organics), poly(triarylamine) (PTAA) and formamidinium iodide (FAI) are all purchased from Xi'an Polymer Light Technology Crop. (China). All the materials were used directly without further purification. Glass/FTO were purchased from Advanced Election Technology Co., Ltd (China).

2. Characterization

The UV-vis absorption spectroscopy was recorded on a Perkin Elmer model Lambda 750 spectrophotometer. The PL spectra were performed by a FluoroMax-4 spectrofluorometer (HORIBA Scientific) with excitation wavelength at 410 nm. TRPL spectra were obtained using a Hamamatsu streak camera. PL data were analyzed on a Nikon 50x objective (N.A. 0.55) in a Nikon ME600 optical microscope. FTIR spectra were collected using a Bruker HYPERION FTIR spectrometer and cumulated 32 scans at a resolution of 4 cm^{-1}. The TEM images were recorded by a Tecnai G2 F20 S-Twin system operated at 200 kV. The fs-TA measurements were performed on a Helios pump-probe system (150 fs, 1 kHz) combined with an amplified femtosecond laser system (excitation wavelength at 400 nm and laser energy of 2 μJ cm^{-2}). The top view and cross-section image were obtained from SEM (a Zeiss G500 with the extra high tension of 10 kV).

J-V curves of the devices carried out at a Keithley 2400 Digital Source Meter under N_2 glovebox and simulated AM 1.5G spectrum at 100 mW cm^{-2} with a solar simulator (Class AAA, 94023A-U, Newport). The active area of 7.25 mm^2 was defined by a shadow mask. The external quantum efficiency (EQE) measurement of the solar cells was measured by a Solar Cell Scan 100 system (Zolix Instruments Co. Ltd.).

3. $CsPbI_3$ QDs synthesis

2 g (6.14 mmol) of Cs_2CO_3 was loaded into a 250 mL three-neck flask along with 8 mL of OA and 100 mL of ODE. After continuous stirring at 90 ^oC under vacuum for 1 hour, the flask was filled with N_2 and heated up to 120 ^oC until $CsCO_3$ completely reacted with OA to form the clarified Cs-oleate. The solution was then transferred to N_2 glovebox and preheated to 100 ^oC to avoid solidification before use.

Meanwhile, 1 g (2.16 mmol) PbI_2 and 50 mL ODE were added into another 250 mL three-neck flask and degassed under vacuum at 90 ^oC for 1 hour with continuous stirring. Then, the switch was converted to N_2 flow, followed by 5 mL of OA and 5 mL of OAm were injected into the flask. Subsequently, the mixture was vacuumed again and maintain the temperature until the PbI_2 was completely dissolved. Then, the reaction system was heated up to 160 ^oC under N_2 atmosphere and 4 mL preheated Cs-oleate was quickly injected. After 5 s, the reaction flask was rapidly quenched to room temperature by an ice bath.

4. $CsPbI_3$ QDs purification

All purification procedures were carried out under a N_2 atmosphere. For the first step purification

process, the crude solution was packed into six centrifuge tubes equally and a triple volume of antisolvent MeOAc was added into it, followed by centrifugation at 8000 rpm for 5 min. Afterward, the precipitate was collected and dissolved in 3 mL hexane for each tube with the supernatant discarded. For the second step purification process, the equal volume MeOAc was added to the solution and centrifuged at 8000 rpm for 3 min. Finally, the purified precipitate was dispersed in 20 mL of hexane total and centrifuged at 4000 rpm for 5 min to remove excess PbI_2 and Cs-oleate. Before use, the supernatant was stored in the dark at 0 ^oC in the refrigerator to precipitate excess Cs-oleate and Pb-oleate.

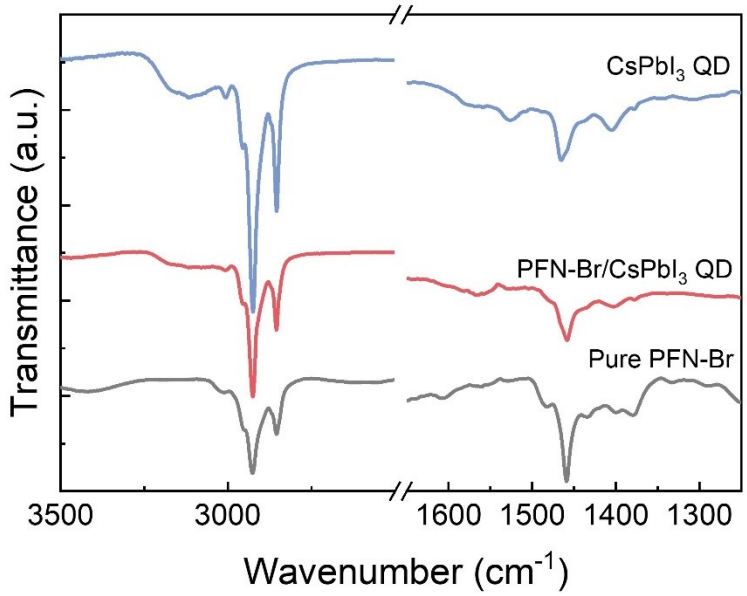

Figure S1. FTIR spectra of $CsPbI_3$ QD, PFN-Br and PFN-Br/$CsPbI_3$ QD.

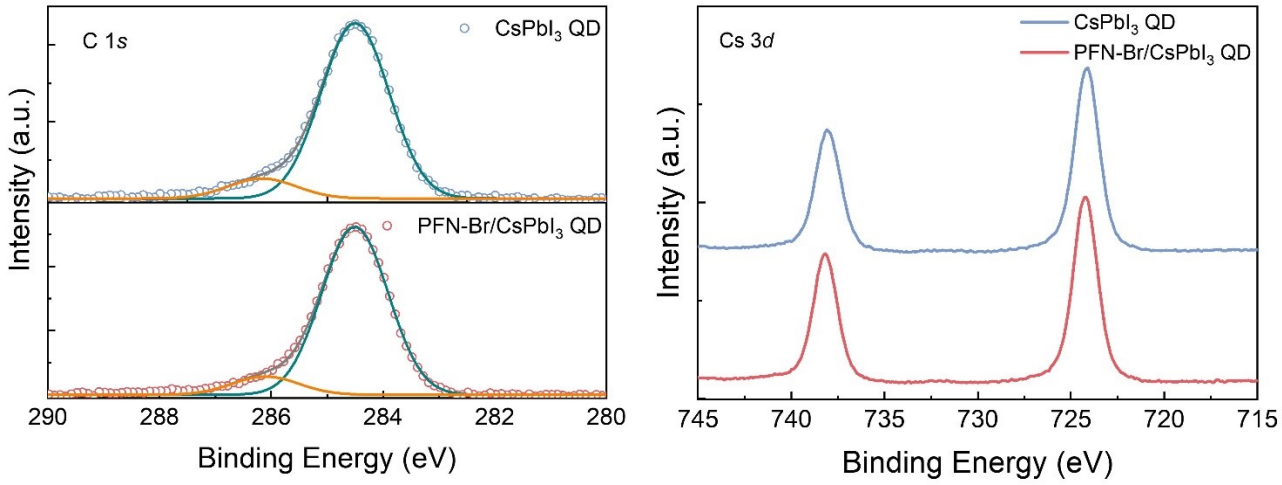

Figure S2. C 1*s* and Cs 3*d* XPS core level spectra of $CsPbI_3$ QD and PFN-Br/$CsPbI_3$ QD.

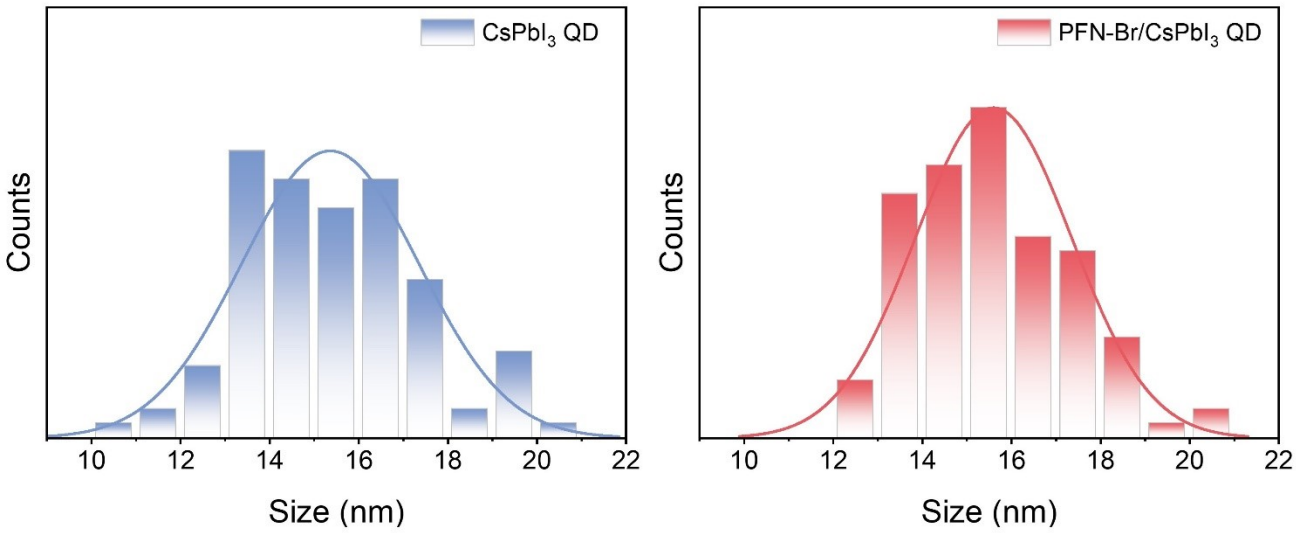

Figure S3. The size distributions of Control and PFN-Br/$CsPbI_3$ QDs.

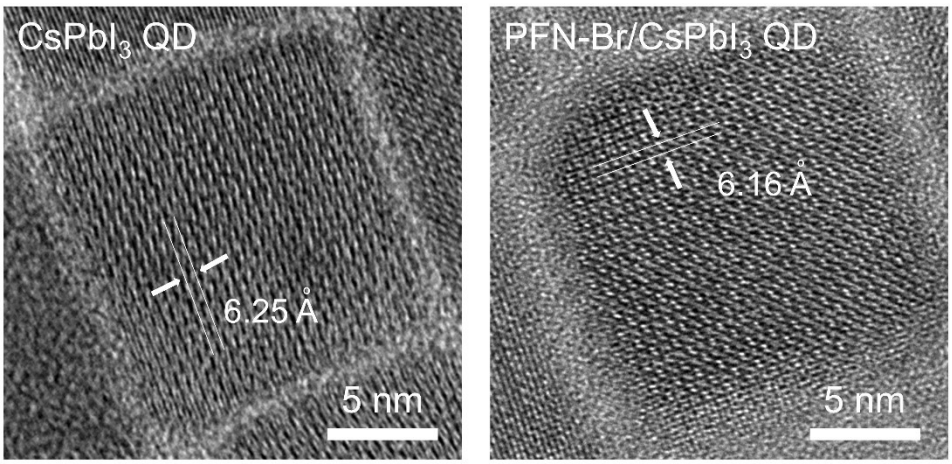

Figure S4. The HRTEM image of $CsPbI_3$ QD and PFN-Br/$CsPbI_3$ QD.

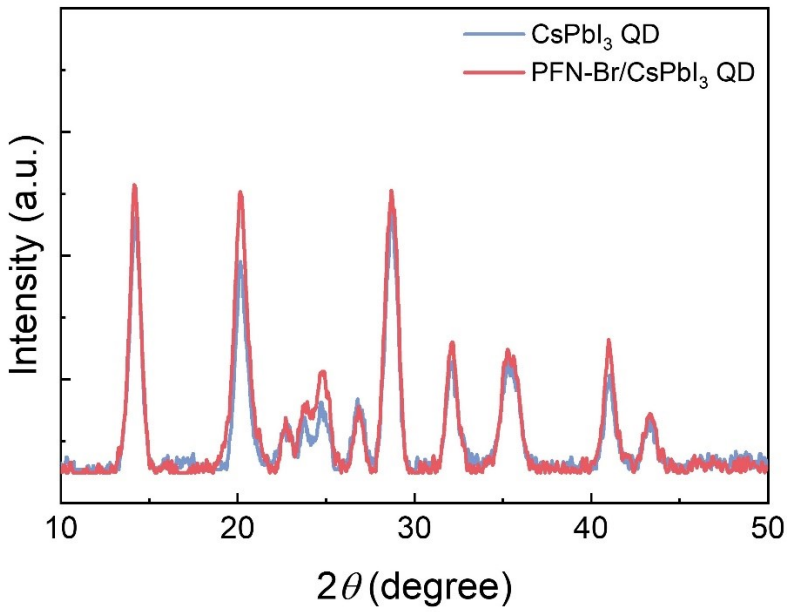

Figure S5. The XRD patterns of $CsPbI_3$ QD and hybrid PFN-Br/$CsPbI_3$ QD films.

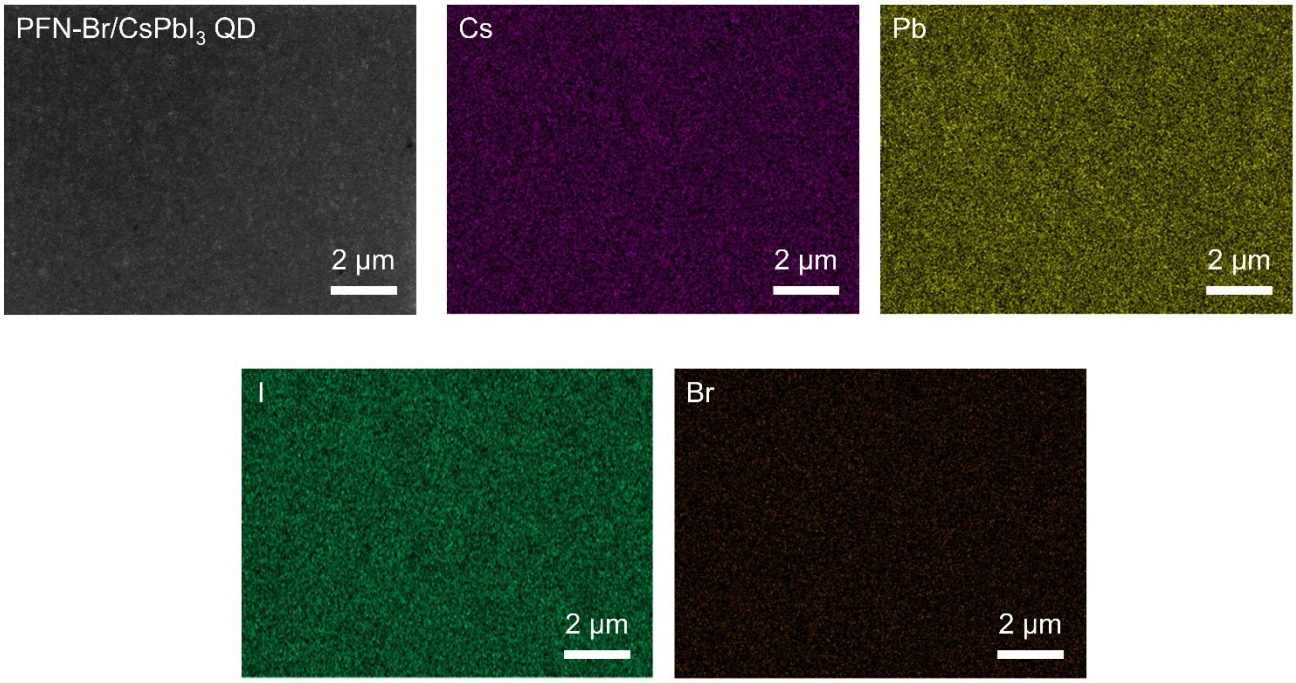

Figure S6. SEM image and the corresponding elemental mappings of the PFN-Br/$CsPbI_3$ QD film.

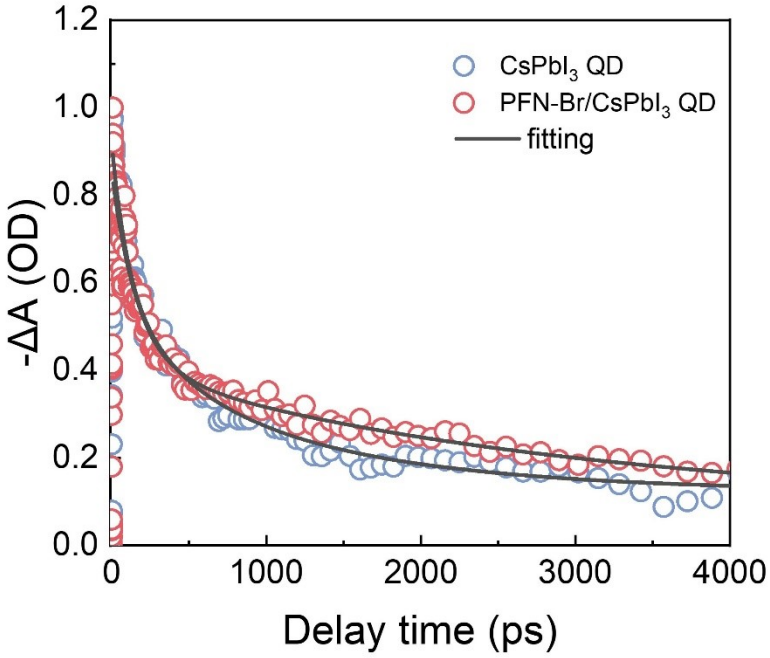

Figure S7. The corresponding GSB decay spectra from the pseudo-colour TA maps.

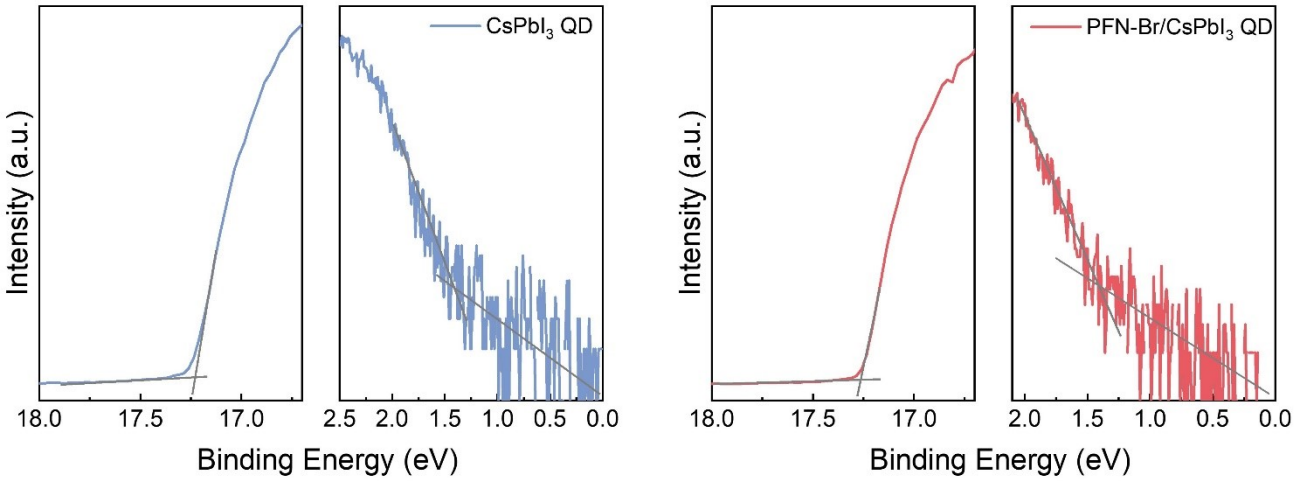

Figure S8. UPS plots of control $CsPbI_3$ QD film and the PFN-Br/$CsPbI_3$ QD film.

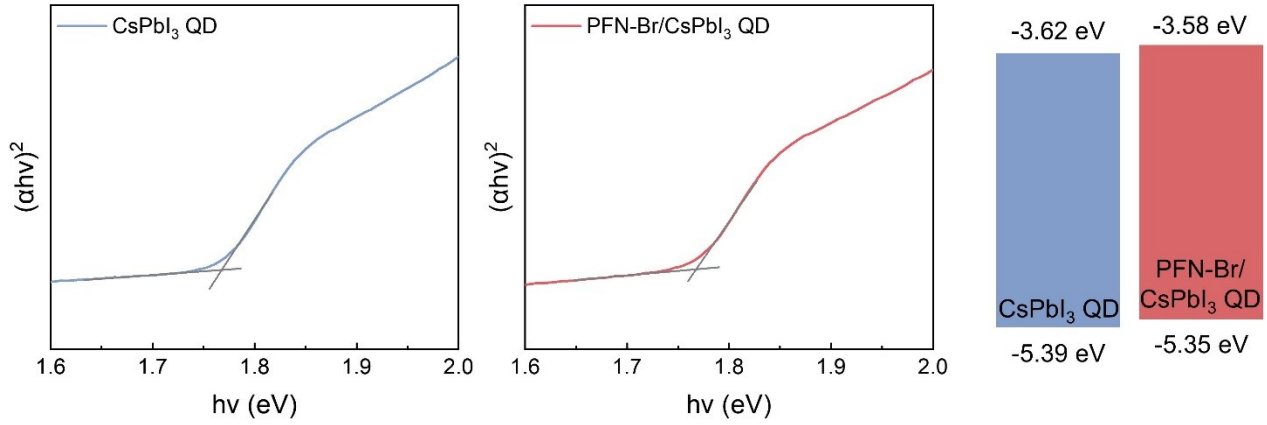

Figure S9. Tauc plots of control and the PFN-Br/$CsPbI_3$ QD films with the energy level diagram of both samples.

Table S1. The detailed parameters of TRPL spectra.

Sample	A_1	τ_1 (ns)	A_2	τ_2 (ns)	τ_{ave} (ns)
$CsPbI_3$ QD	41.2	0.77	58.8	10.15	1.68
PFN-Br/$CsPbI_3$ QD	13.4	0.98	86.6	16.31	5.31

Table S2. Tri-exponential fitting parameters of TA delay data.

Sample	τ_1 (ps)	τ_2 (ps)	τ_3 (ps)
$CsPbI_3$ QD	106.74107	438.72	1354.45
PFN-Br/$CsPbI_3$ QD	164.446	473.24	2993.08

Table S3. The detailed device parameters extracted from *J-V* curves of $CsPbI_3$ PQD solar cells

Condition	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
$CsPbI_3$ QD	1.232	14.96	0.72	13.31
PFN-Br/$CsPbI_3$ QD	1.251	16.22	0.74	15.07