

Electronic Supplementary Information (ESI)

**Efficient and Stable CsPbI<sub>3</sub> Perovskite Quantum Dots Enabled by *in-situ* Ytterbium Doping for Photovoltaic Application**

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## 1. Characterizations:

UV-Vis spectra were recorded on a Perkin Elmer model Lambda 750. Powder XRD patterns were recorded by using a Rigaku D/Max-Ra X-ray diffractometer with a monochrome at Cu K $\alpha$  radiation ( $\lambda = 1.54178\text{\AA}$ ). The morphologies of the CsPbI<sub>3</sub> Quantum Dots (QDs) were characterized by using a TEM (Tecnai G2 F20 S-Twin transmission electron microscope) operated at 200 kV. TEM samples were prepared by drop casting the solution on a carbon-coated copper grid. Time-resolved PL spectra were detected using a Hamamatsu streak camera. PL and PLQY data were collected using a Nikon 50x objective (N.A. 0.55) in a Nikon ME600 optical microscope. XPS measurements were carried out using an XR6 monochromated AlK $\alpha$  X-ray source ( $h\nu = 1486.6\text{ eV}$ ) with a 900  $\mu\text{m}$  spot size and a 20 eV pass energy. The TRPL decay lifetimes were acquired via a Monochromator/Spectrograph (Omni -  $\lambda 300$ , Zolix) and an Oscilloscope (GDS-3354, GWINSTEK). The 365 nm excitation pulses were generated from an optical parametric amplifier (TOPAS-800-fs), pumped by the Coherent Legend regenerative amplifier (35 fs, 1 Hz, 800 nm), and seeded by a Coherent Vitesse oscillator (30 fs, 80 MHz).

## 2. Synthesis of Cs-oleate Solution

0.5 g of Cs<sub>2</sub>CO<sub>3</sub> powder, 2 mL of Oleic Acid (OA), and 50 mL of 1-Octadecene (ODE) were loaded into a 100 mL three-neck round-bottom flask. The solution was then vacuumed for 60 minutes at 80 °C and heated to 120 °C under N<sub>2(g)</sub> until all the Cs<sub>2</sub>CO<sub>3</sub> reacted with OA to form the cesium-oleate (Cs-oleate) precursor. In ODE and an N<sub>2(g)</sub> environment, the Cs-oleate was stored and heated to 100 °C and is ready for use in the synthesis of the CsPbI<sub>3</sub> QDs.

## 3. Isolation and purification of obtained CsPbI<sub>3</sub> QDs

During the isolation process, Methyl Acetate (MeOAc) was used to extract the cubic phase of the CsPbI<sub>3</sub> QDs. The synthesized QDs were separated into two centrifugal tubes and then subsequently divided again into three more, leaving six tubes of equal volume. After adding 32 mL of MeOAc to each tube (ratio of QD

reaction solution to MeOAc is 1:3) they were centrifuged at 8000 RPM for five minutes. The generated precipitate in each centrifugal tube was redispersed in 3 mL of hexane. The solutions of three tubes were collected into one, resulting in two tubes of equal volume. 9 mL of MeOAc was then added to both tubes which were then centrifuged at 8000 RPM for three minutes. The QDs were then redispersed in 20 mL of hexane and centrifuged again at 4000 RPM for five minutes to remove excess unreacted precursor such as the Pb-oleate. The supernate was reserved at 0 °C for 12 hours in a dark environment to further precipitate excess Cs-oleate and Pb-oleate. After the solution had recovered to room temperature, the QDs are centrifuged again at 4000 RPM for five minutes to obtain the final product for fabricating the solar cells devices.

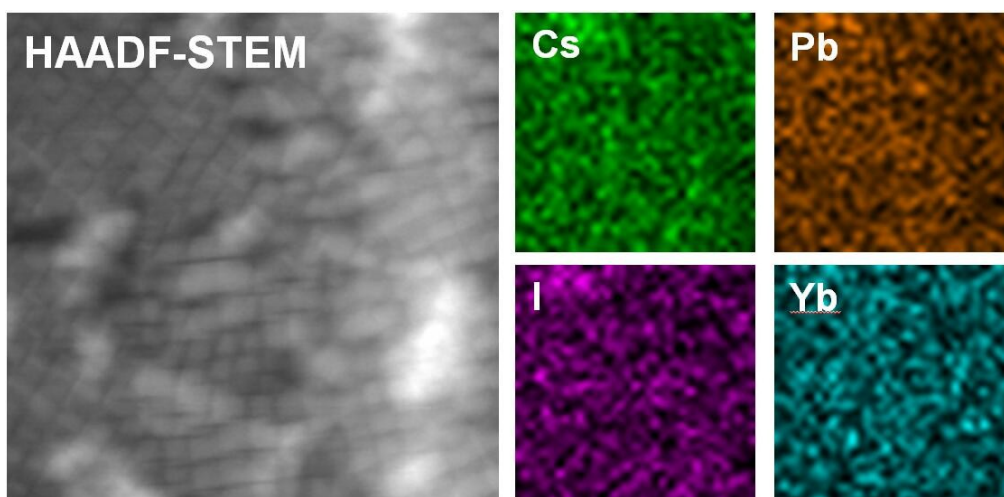


Figure S1. HAADF-STEM images and the elemental mappings of Cs, Pb, I and Yb for 20% Yb-doped CsPbI<sub>3</sub> QDs.

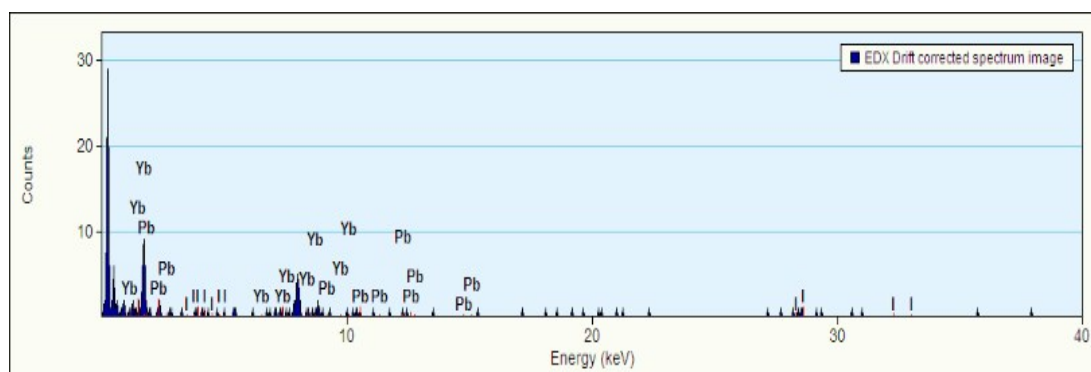


Figure S2. The EDX spectrum of 20% Yb-doped CsPbI<sub>3</sub> QDs.

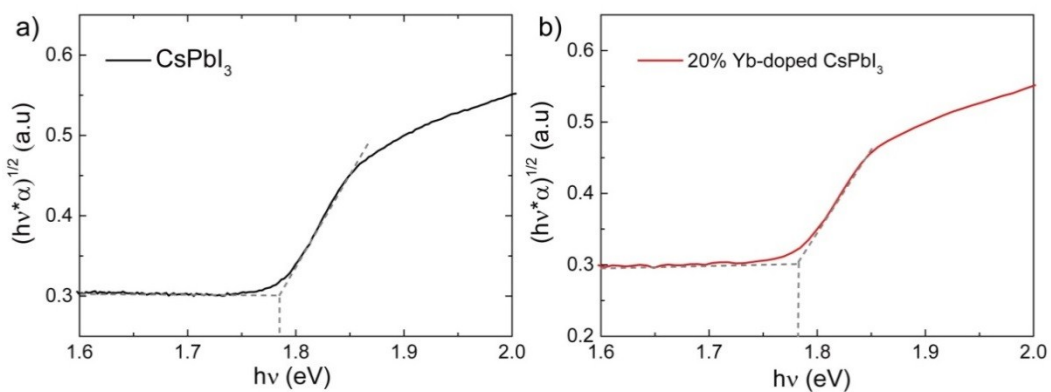


Figure S3. Tauc plots of absorbance with photon energy ( $h\nu$ ) and extracted bandgaps of  $\text{CsPbI}_3$  ( $1.773 \pm 0.003$  eV) and 20% Yb-doped ( $1.753 \pm 0.003$  eV)  $\text{CsPbI}_3$  QD film.

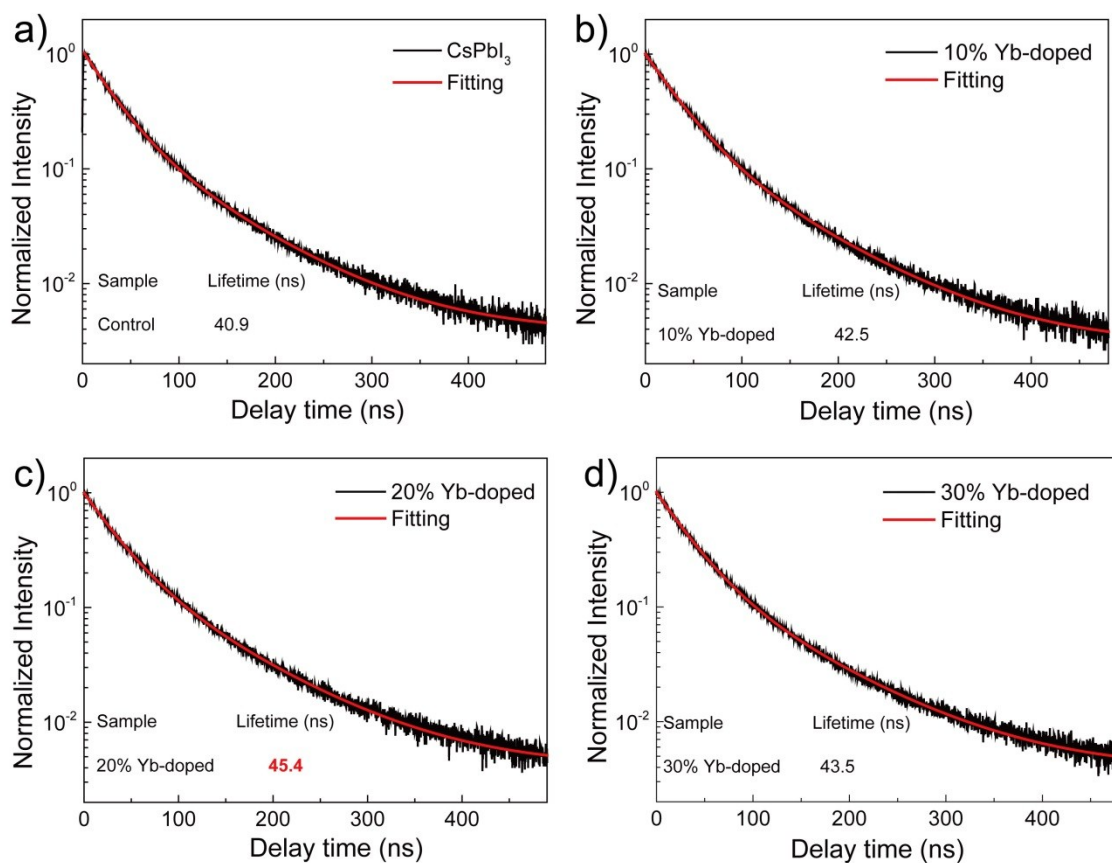


Figure S4. Time-resolved PL characteristics of the  $\text{CsPbI}_3$  (a), 10% Yb-doped (b), 20% Yb-doped (c) and 30% Yb-doped (d)  $\text{CsPbI}_3$  QD solutions.

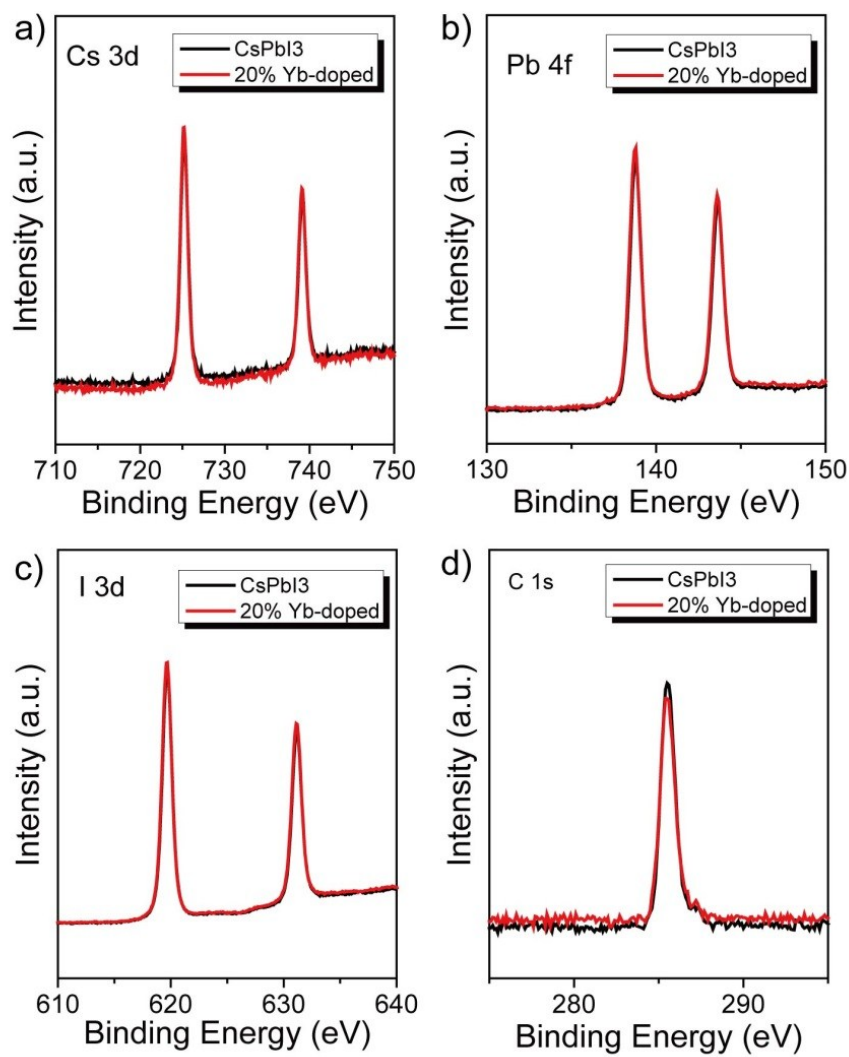


Figure S5. The core level spectra of Cs (a), Pb (b), I (c) and C (d) from XPS spectra for CsPbI<sub>3</sub> and 20% Yb-doped CsPbI<sub>3</sub> QDs film.

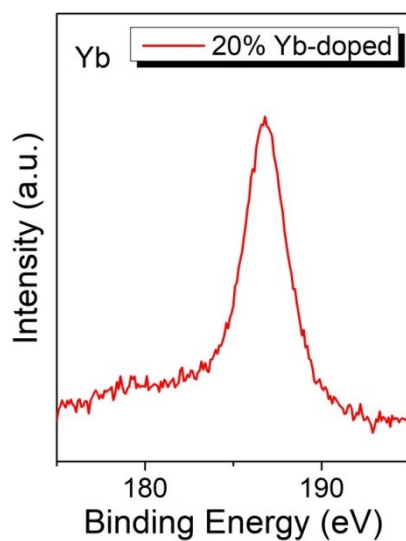


Figure S6. The core level spectra of Yb from XPS spectra for 20% Yb-doped CsPbI<sub>3</sub> QDs

film

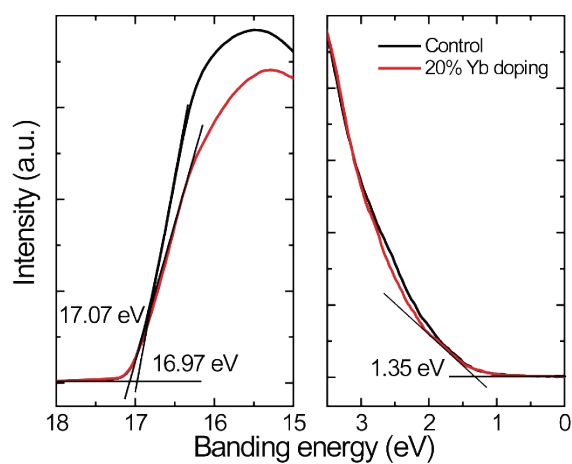


Figure S7. UPS spectra of CsPbI<sub>3</sub> and 20% Yb-doped CsPbI<sub>3</sub> QD film, the left panel of each show the secondary electron cut-off region and the right panel shows the magnified spectra near Fermi edge.

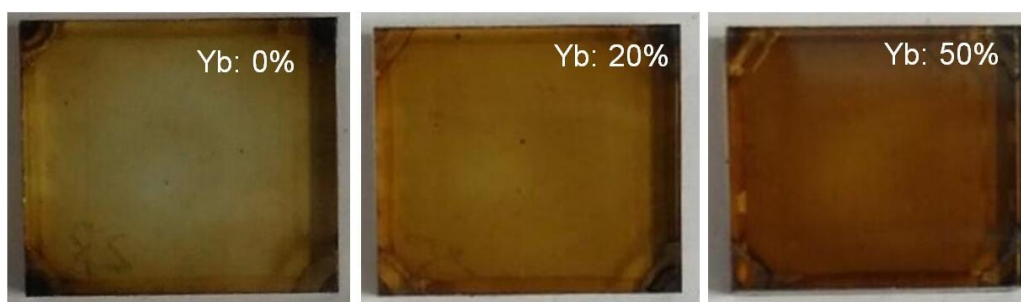


Figure S8. Images of the corresponding CsPbI<sub>3</sub> QD films after 7 days under the ambient environment with a 20-30% relative humidity at room temperature.

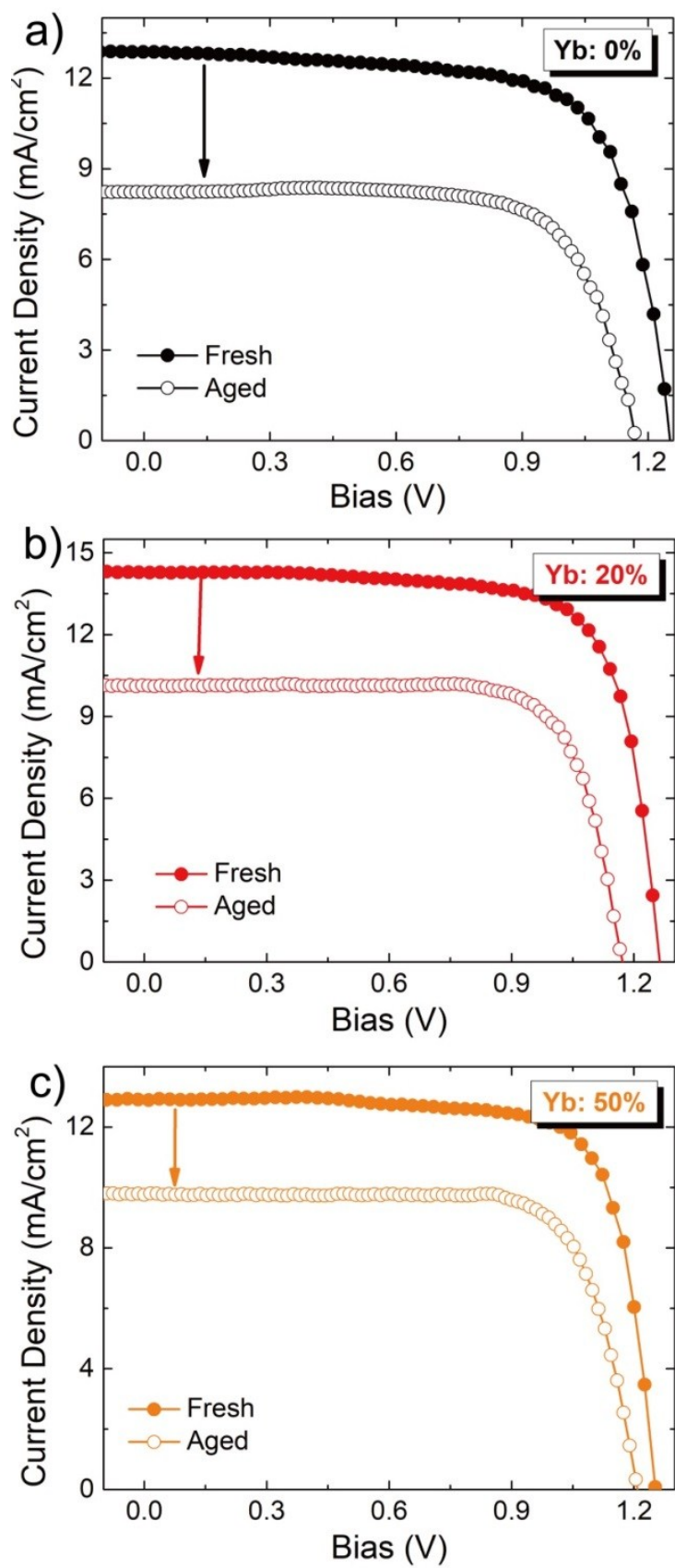


Figure S10. The J-V curves of the fresh devices and after 7 days storage under ambient condition based on CsPbI<sub>3</sub> QD with different Yb-doping contents.

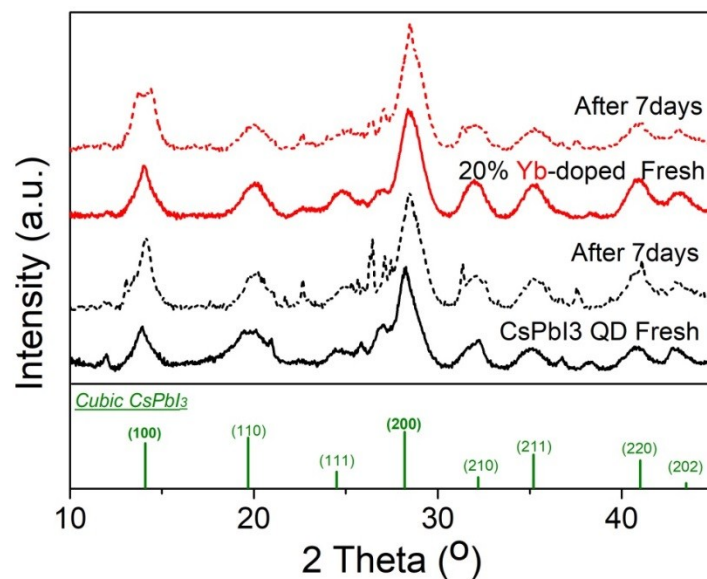


Figure S9. XRD patterns before and after 7 days of corresponding films on FTO/TiO<sub>2</sub> substrate, which were exposed to ambient conditions (Temperature: ~20%; relative humidity: 20-30%).

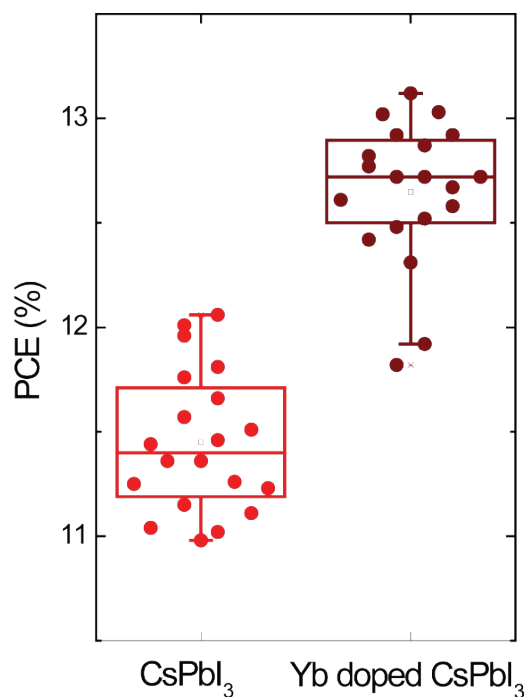


Figure S11. PCE distribution histograms of pristine CsPbI<sub>3</sub> and 20% Yb-doped CsPbI<sub>3</sub> QDs based solar cells based on 20 parallel devices.



Table S1. The fitting results of pristine and 20% Yb-doped CsPbI<sub>3</sub> QD solution 1D TRPL fitting detail.

	$A_1$	$t_1$ (ns)	$A_2$	$t_2$ (ns)	$T_{Average}$ (ns)
0% Yb-doped	0.3365	94.98233	0.6635	34.87677	44.3
20% Yb-doped	0.4182	114.2228	0.5818	36.84849	51.4

Table S2. Devices parameters extracted from  $J$ - $V$  scans after 7 days storage under ambient condition

	$V_{oc}$ (V)	$J_{sc}$ (mA/cm <sup>2</sup> )	$FF$ (%)	PCE (%)
0% Yb-doped	1.18	8.31	0.62	6.16
20% Yb-doped	1.18	10.10	0.74	9.21
50% Yb-doped	1.20	9.85	0.76	8.98