Electronic Supplementary Information

Pure Red Emitting Composites with Nearly 100% Solid–state Photoluminescence Quantum Yield Obtained by In-situ Growth Sr^{2+}-doped Hybrid Halides $CsPb(Br,I)_3$ Perovskite Quantum Dots in Mesoporous Silica

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Experiment Section

Materials and Chemicals. Cesium carbonate (Cs_2CO_3, Aladdin, 99.9%), lead bromide ($PbBr_2$, Aladdin, 99.0%), lead iodide (PbI_2 99.0%), strontium iodide hexahydrate ($SrI_2 \cdot 6H_2O$, Aladdin, 99.99%) and oleylamine (OAm, Aladdin, 80–90%), 1-octadecene (ODE, Sigma Aldrich, 90%), and oleic acid (OA, Sigma Aldrich, 90%) , mesoporous silica (SBA-15, from Jiangsu XFNANO Materials Technology Co., 99%). All chemicals were used without further purification.

Preparation of Cs−Oleate. Cs_2CO_3 (0.814 g), OA (2.5 mL), and ODE (40 mL) were added into a 50 mL three-necked flask and dried for 10 mins at 130 °C, and the mixture was then heated to 150 °C under N_2 to totally dissolve the Cs_2CO_3 powder. Since Cs-oleate precipitates out of ODE at room temperature, it has to be preheated to 150 ºC before injection.

Synthesis of $CsPb(Br_{1-x}I_x)_3$ PeQDs. 0.188 mmol lead halide ($PbBr_2$ and PbI_2) and ODE (5ml) were loaded into a 50 mL 3-neck flask and dried under vacuum at 120 ºC for 1h, then 0.5 mL of dried OAm and 0.5 mL of dried OA were injected at 120 ºC under N_2. After the complete dissolution of lead halide, the temperature of the precursor was raised to 180°C and held, then 0.4 mL of Cs-oleate precursor was injected rapidly, and 10s later the reaction mixture was immediately cooled down to room temperature by immersion in a cold-water bath.

Synthesis of Sr^{2+} doped $CsPb(Br_{0.4}I_6)_3$ PeQDs. All the steps were the same as those for the synthesis of $CsPb(Br_{0.4}I_{0.6})_3$ PeQDs, except for the addition of a certain amount of SrI_2 to the lead halide ($PbBr_2$ and PbI_2) before the injection of precursor solution. During the synthesis, the amount of $PbBr_2$ was fixed at 0.0752 mmol, and the total amount of PbI_2 and SrI_2 is fixed at 0.1108 mmol.

Purification of PeQDs. The PeQDs solution was separated at 10000 rpm for 5 minutes. The bottom precipitate was taken out and dispersed in 5 ml cyclohexane, followed by another 6000rpm core separation for 3 min. The bottom precipitate was again dispersed in anhydrous hexane for subsequent characterization tests.

Synthesis of $CsPb(Br_{0.4}I_6)_3$:20%Sr^{2+}@m-SiO_2 composite. The synthesis $CsPb(Br_{0.4}I_6)_3$:20%Sr^{2+}@m-SiO_2 composite was performed in the same way as that of synthesis of $CsPb(Br_{0.4}I_6)_3$:20%Sr^{2+} PeQDs, with the only difference being that 2.444 mmol mesoporous silica was firstly dissolved in a mixed solution (5 mL ODE, 0.5 ml OA and 0.5 ml OAm), and then 0.0752 mmol $PbBr_2$, 0.0752 mmol PbI_2 and 0.0376 mmol SrI_2 were added and dissolved in the same solution before the injection of precursor solution. After cooling down, the mixture solution was centrifuged at 3000 rpm for 3 min, and the primary precipitation was dispersed in 14 ml of hexane solution, then left for 2h to get the secondary precipitation, and finally the secondary precipitation was dried under vacuum for further characterization.

Characterization. The phase purity of the samples was analyzed by powder X-ray diffraction (XRD) using a Bruker D2 phaser X-ray diffractometer with Cu Kα radiation (λ=1.54056 Å, 30 kV, 15 mA). The morphology of all samples were investigated using transmission electron microscopy (TEM) at an operating voltage of 300kV (Tecnait G2F30, FEI, USA). X-ray photoelectron spectra (XPS) were performed on a Kratos AXIS Ultra-DLD spectrometer. Fourier transform infrared spectra (FTIR) were obtained via the KBr pellet method using a Thermo Nicolet 6700 spectrophotometer. Photoluminescence spectra were measured by an Edinburg FS-5 spectrophotometer equipped with a 450 W xenon lamp. The absolute PLQYs were measured by an absolute PLQY spectrometer (C9920-03, Hamamatsu). Time resolved decay curves were taken on an Edinburgh FLS 980 spectrometer using a picosecond pulsed light emitting diode (EPLED 360) as the light source.

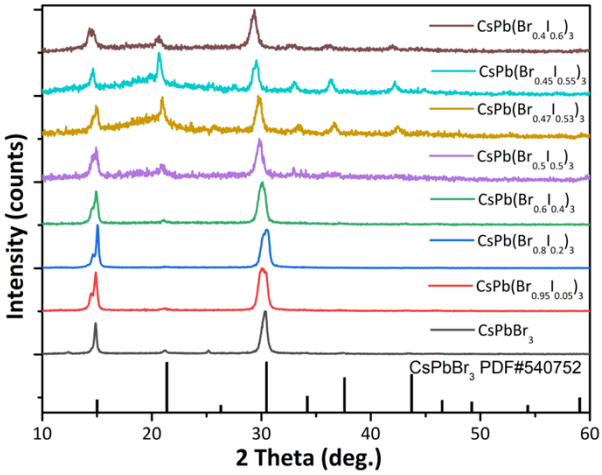

Fig. S1 XRD pattern of $CsPb(Br_{1-x}I_x)_3$ ($0 \le x \le 60\%$) PeQDs

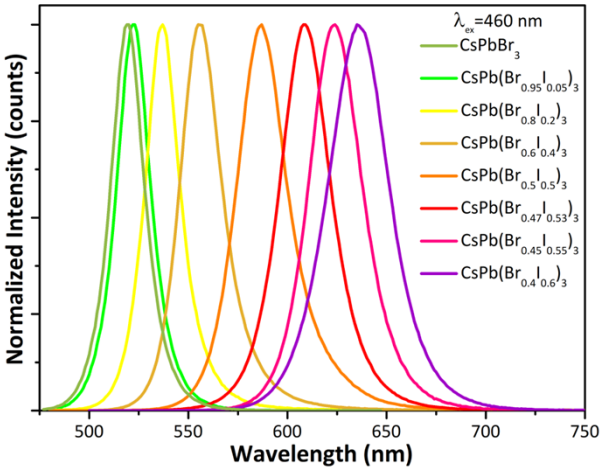

Fig. S2 PL spectra of $CsPb(Br_{1-x}I_x)_3$ ($0 \le x \le 60\%$) PeQDs

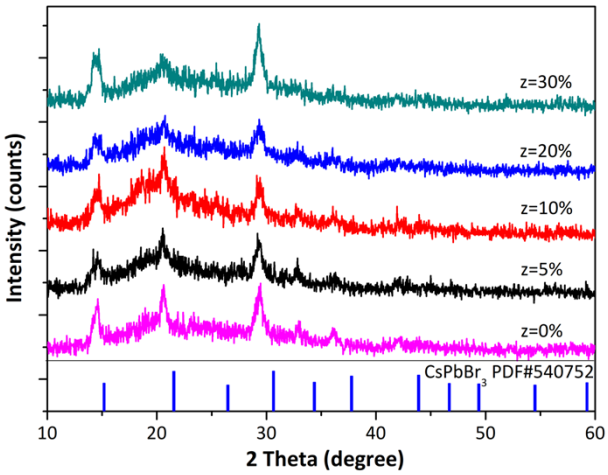

Fig. S3 XRD pattern of $CsPb_{1-z}(Br_{0.4}I_{0.6})_3{:}zSr^{2+}$ ($0 \le z \le 30\%$) PeQDs

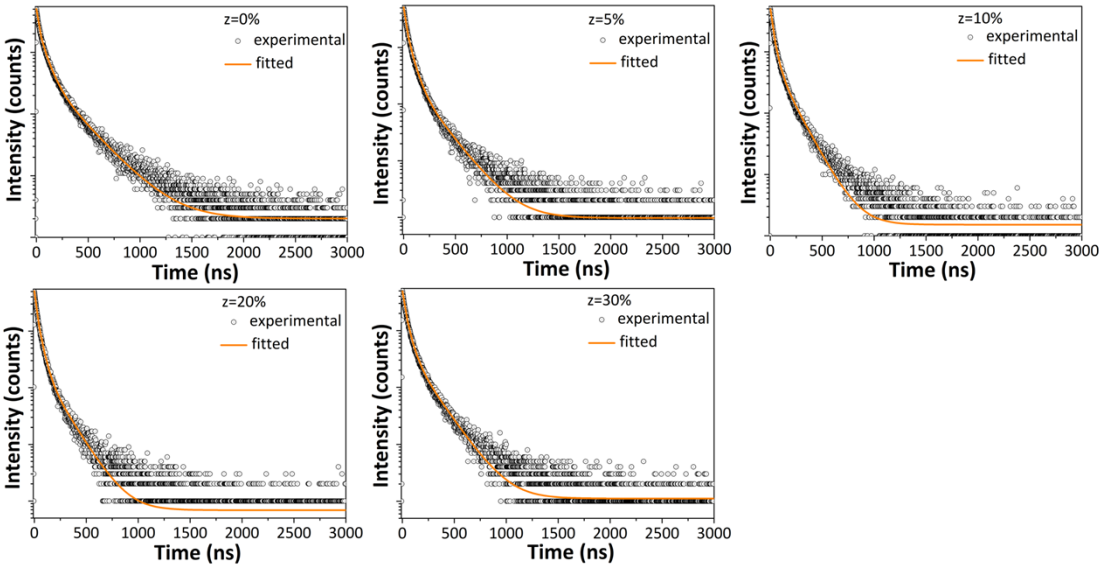

Fig. S4 Decay curves of $CsPb_{1-z}(Br_{0.4}I_{0.6})_3$:$zSr^{2+}$ ($0 \leq z \leq 30\%$) PeQDs with fitted lines.

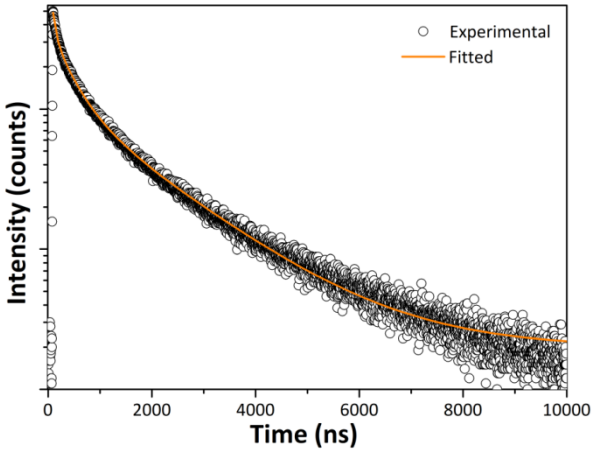

Fig. S5 Decay curves of $CsPb_{1-z}(Br_{0.4}I_{0.6})_3$:$20\%Sr^{2+}$ @m-SiO_2 composite with fitted lines.

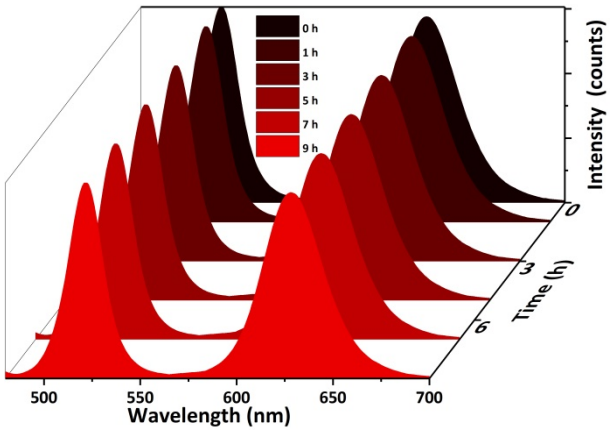

Fig. S6 PL spectra of $CsPbBr_3$ @m-SiO_2 composites and $CsPb(Br_{0.4}I_{0.6})_3$:$20\%Sr^{2+}$@m-SiO_2 composite mixtures measured at different times.