

Electronic Supplementary Information

CsPbBr₃ and CsPbI₃ rhombic dodecahedra and nanocubes displaying facet-dependent optical properties

Ya-Chu Yang, Yun-Wen Peng, An-Ting Lee, Gautam Kumar and Michael H. Huang*

Department of Chemistry and Frontier Research Center on Fundamental and Applied Sciences of Matters, National Tsing Hua University, Hsinchu 30013, Taiwan

Table of contents

Fig. S1	Illustration of the CsPbBr ₃ crystal synthesis process and the reagent amounts used	2
Fig. S2	SEM images showing the formation of CsPbBr ₃ octahedra	2
Fig. S3	Size distribution histograms of the synthesized CsPbBr ₃ crystals	3
Fig. S4	XRD patterns of the synthesized CsPbBr ₃ crystals	4
Fig. S5	Photographs of the CsPbBr ₃ particle solutions	4
Fig. S6	UV-vis spectrum of the prepared CsPbBr ₃ nanocube solution.	5
Fig. S7	UV-vis absorption spectra of the synthesized CsPbBr ₃ rhombic dodecahedra with tunable sizes and their Tauc plots	5
Fig. S8	Size distribution histograms of the prepared CsPbI ₃ nanocubes	5
Fig. S9	XRD pattern of the synthesized CsPbI ₃ nanocubes.	6
Fig. S10	Photographs of the CsPbBr ₃ solution undergoing anion exchange reaction	6
Fig. S11	SEM image of the 130 nm CsPbBr ₃ rhombic dodecahedra	7
Fig. S12	UV-vis absorption and photoluminescence spectra of the anion-exchanged CsPbBr ₃ rhombic dodecahedra	7
Fig. S13	SEM images of a CsPbBr ₃ rhombic dodecahedron and the converted CsPbI ₃ rhombic dodecahedron	8
Fig. S14	Photographs of the CsPbI ₃ solution undergoing anion exchange reaction	8
Fig. S15	SEM image of CsPbI ₃ nanocubes and the converted CsPbBr ₃ nanocubes	8

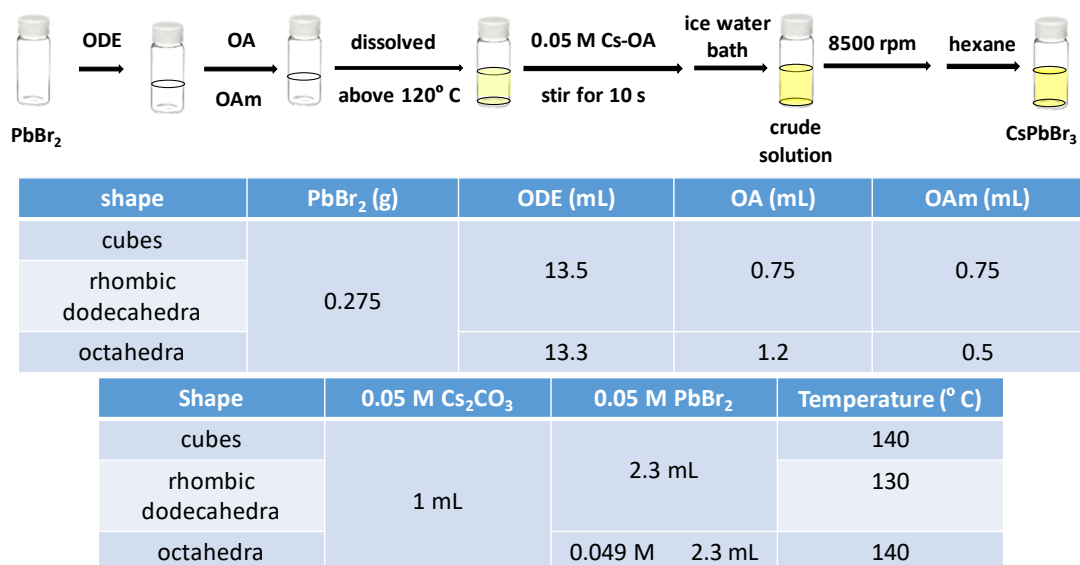


Fig. S1 Schematic illustration of the CsPbBr₃ crystal synthesis process and the reagent amounts used. Again the rate of bringing the frozen solid back to room temperature is critical to size control of rhombic dodecahedra. For 59 nm rhombic dodecahedra, melting took about 2 min, and around 5 and 10 min to make 80 and 168 nm rhombic dodecahedra, respectively.

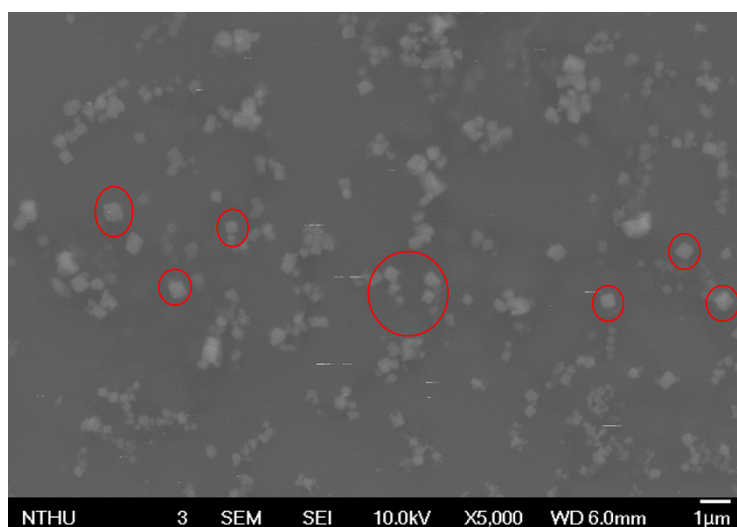


Fig. S2 Additional SEM images showing the formation of CsPbBr₃ octahedra. The circles indicate examples of octahedra.

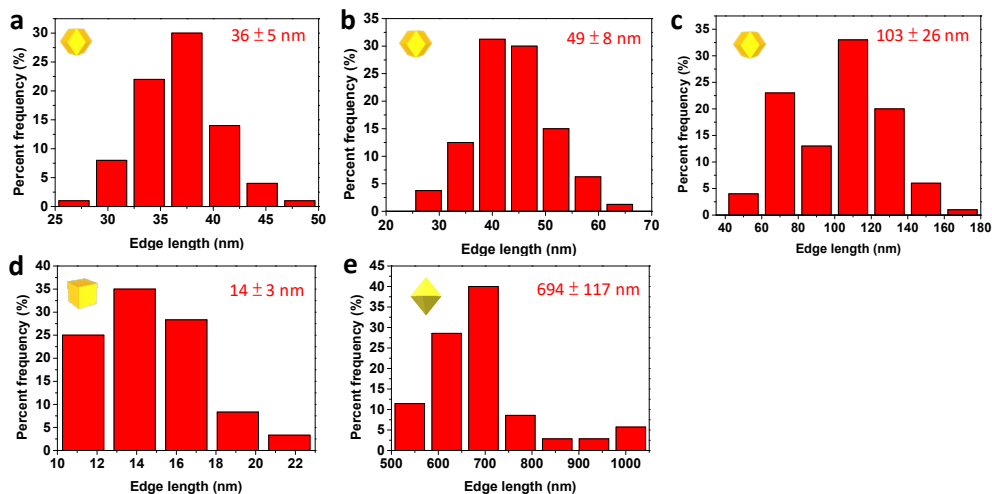


Fig. S3 Size distribution histograms of the synthesized (a) 59, (b) 80, and (c) 160 nm CsPbBr_3 rhombic dodecahedra, (d) nanocubes, and (e) octahedra. From average edge length, the average opposite face length of rhombic dodecahedra is determined. The opposite corner distance of octahedra can be obtained from the average edge length.

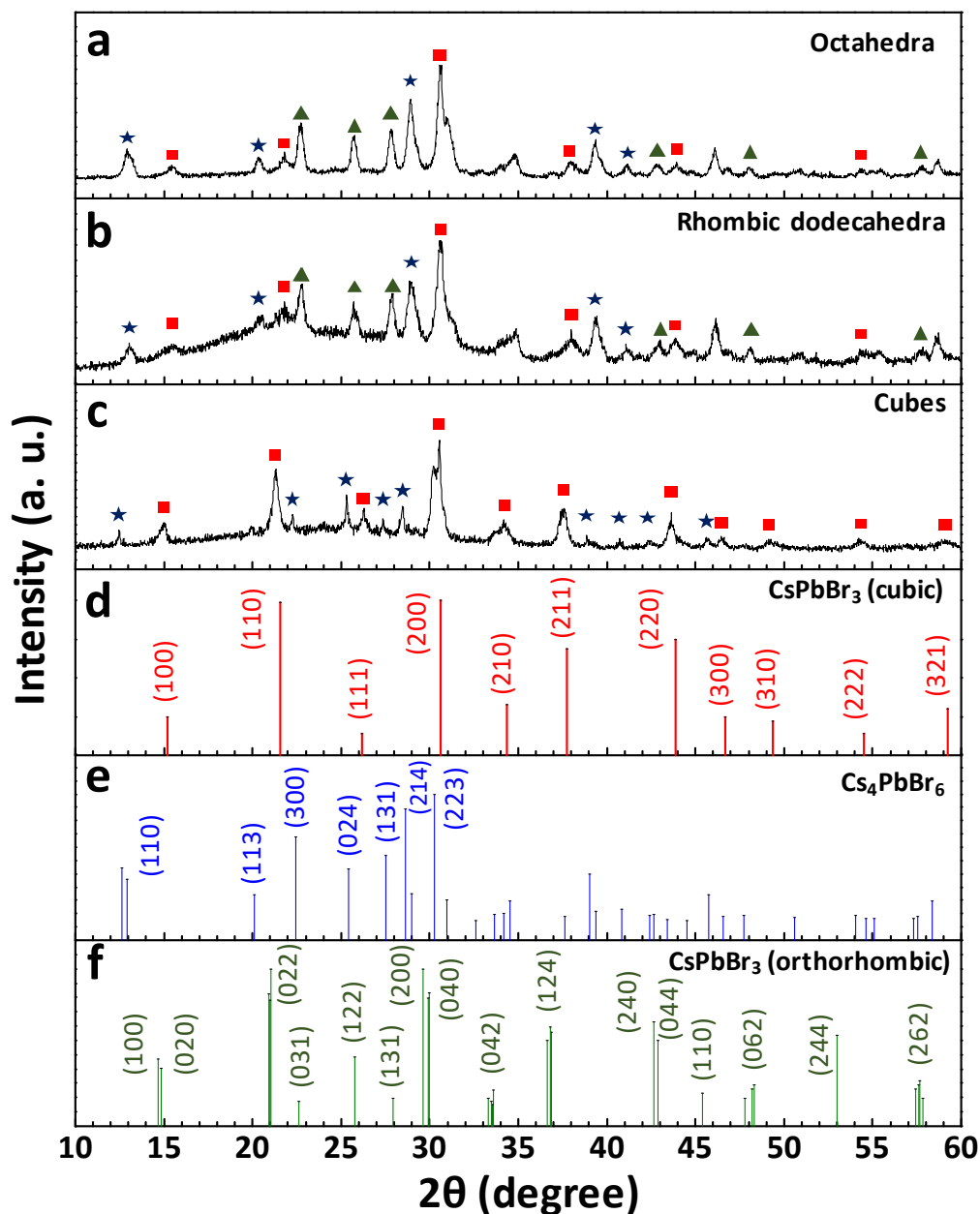


Fig. S4 XRD patterns of the synthesized CsPbBr_3 (a) octahedra, (b) 59 nm rhombic dodecahedra, (c) nanocubes, (d) standard cubic CsPbBr_3 (squares), (e) Cs_4PbBr_6 (stars), and (f) orthorhombic CsPbBr_3 (triangles). A few peaks do not exactly match to any of the possible crystal phases.

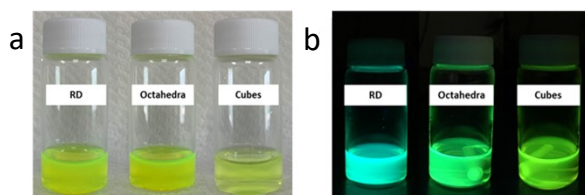


Fig. S5 Photographs of the CsPbBr_3 particle solutions (a) under room light and (b) illuminated by UV light.

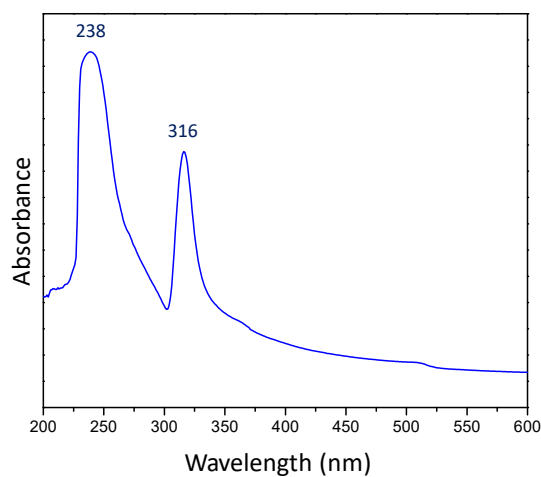


Fig. S6 Room-temperature UV-vis spectrum of the prepared CsPbBr₃ nanocubes in hexane. Significant bands from Cs₄PbBr₆ are present. The CsBrBr₃ absorption band is also observable.

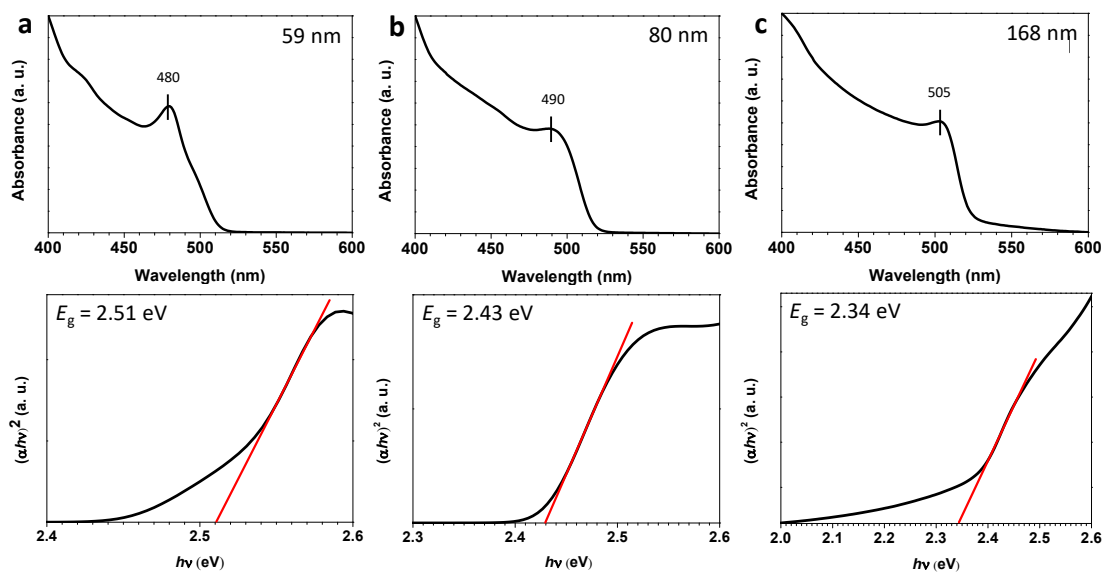


Fig. S7 (a–c) Room-temperature UV-vis absorption spectra of the synthesized CsPbBr₃ rhombic dodecahedra with tunable sizes dispersed in hexane. (d–f) Tauc plots for rhombic dodecahedra with opposite face lengths of 59, 80, and 168 nm.

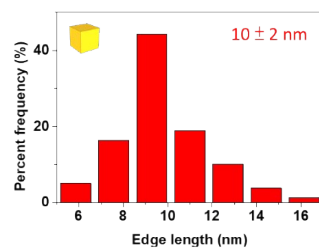


Fig. S8 Size distribution histograms of the prepared CsPbI₃ nanocubes.

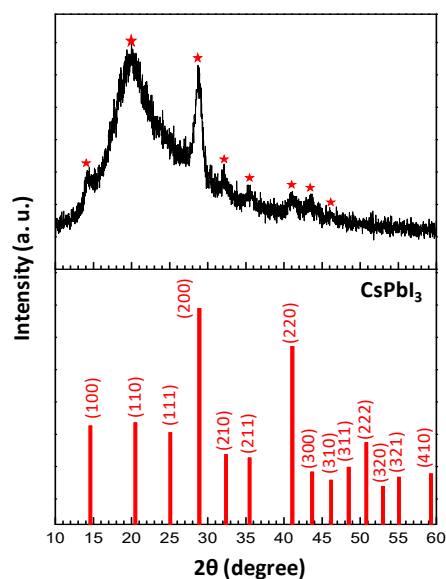


Fig. S9 XRD pattern of the synthesized CsPbI₃ nanocubes. Standard XRD pattern is also shown.

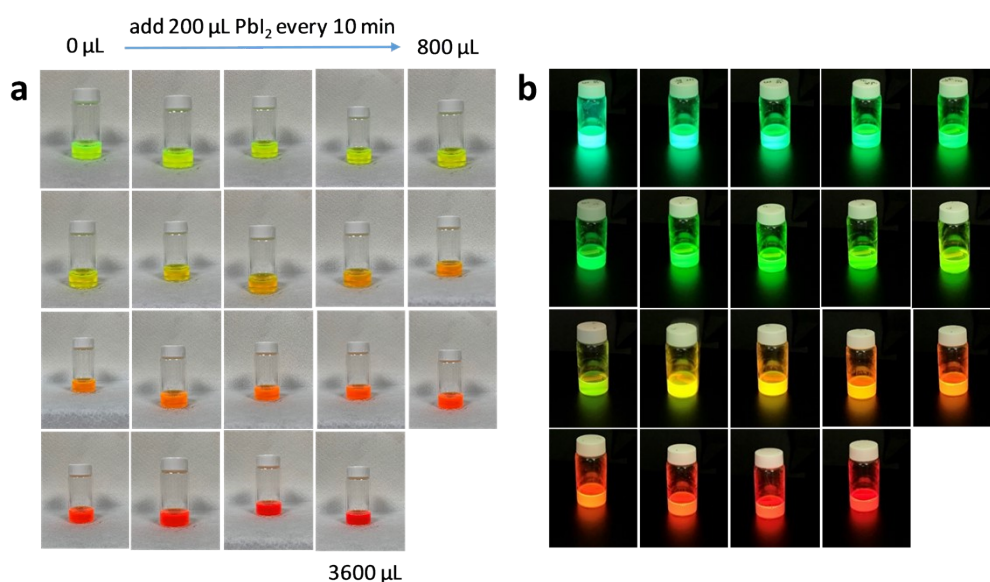


Fig. S10 Digital photographs of the CsPbBr₃ solution undergoing anion exchange reaction under (a) room light and (b) UV lamp illumination ($\lambda = 365$ nm). From left to right and top to bottom, the photos show the solution color changes with sequential addition of 200 μ L of PbI₂ solution every 10 min.

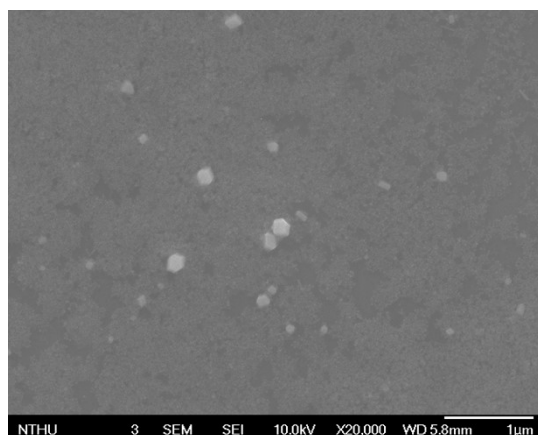


Fig. S11 SEM image of the synthesized 130 nm CsPbBr₃ rhombic dodecahedra.

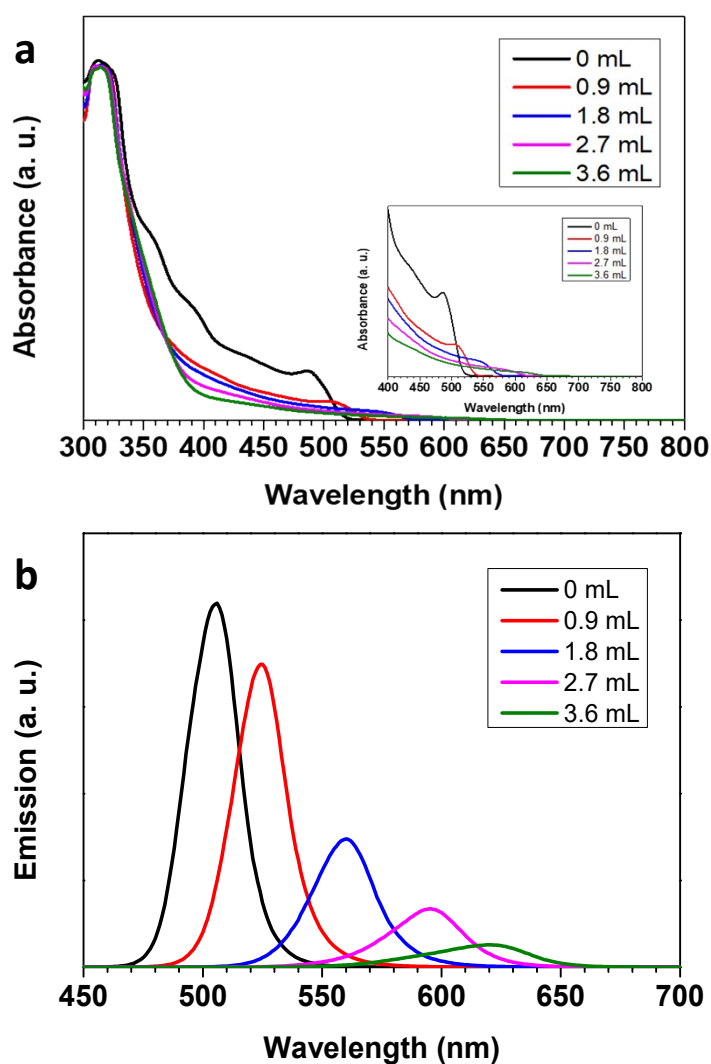


Fig. S12 (a) Room-temperature UV-vis absorption spectra of the anion-exchanged CsPbBr₃ rhombic dodecahedra with addition of different volumes of PbI₂ solution. Inset shows an expanded view. (b) Photoluminescence spectra of the same solutions.

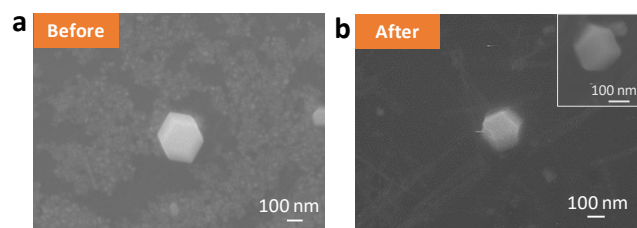


Fig. S13 SEM images of (a) a CsPbBr_3 rhombic dodecahedron and (b) the converted CsPbI_3 rhombic dodecahedron.

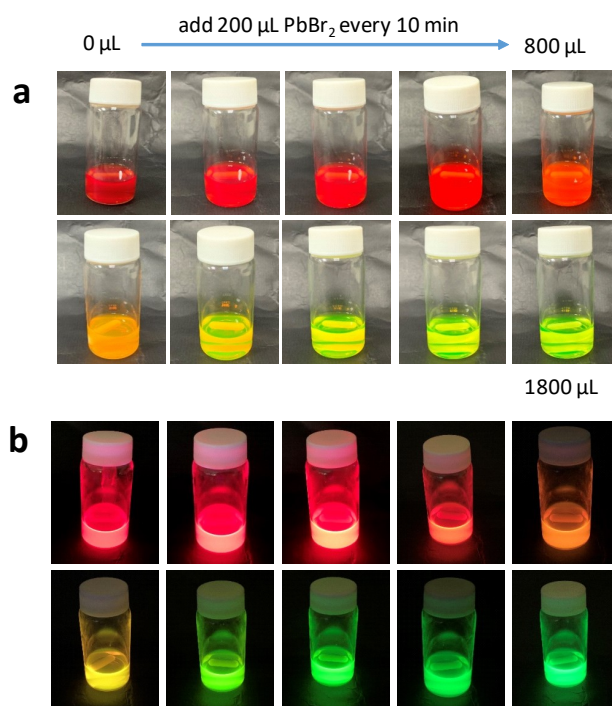


Fig. S14 Digital photographs of the CsPbI_3 solution undergoing anion exchange reaction under (a) room light and (b) UV lamp illumination. From left to right, the photos show the solution color changes with sequential addition of 200 μL of PbBr_2 solution every 10 min.

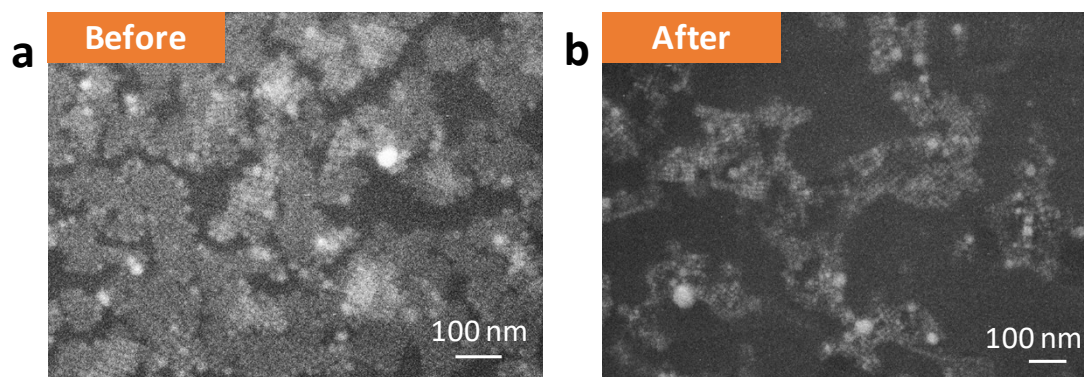


Fig. S15 (a) SEM image of CsPbI_3 nanocubes and (b) the converted CsPbBr_3 nanocubes.