

Electronic Supplementary Information

Exploring optimal *in-situ* fabrication conditions to realize core–shell CsPbBr₃ QDs with high PLQYs and structural stabilities by dual-defect passivation[‡]

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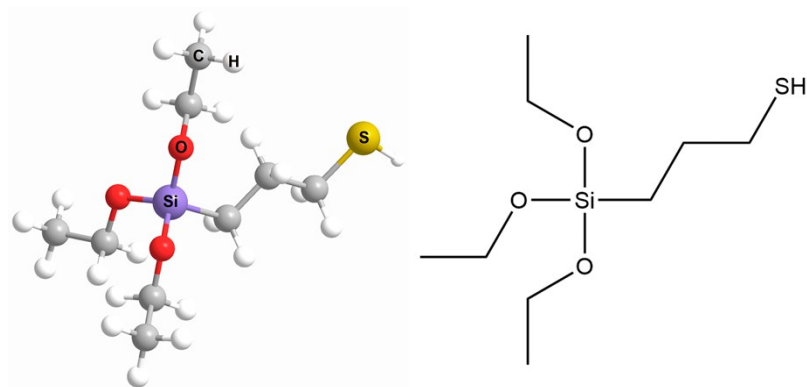


Figure S1. Molecular structure of (3-mercaptopropyl)triethoxysilane (MPTES).

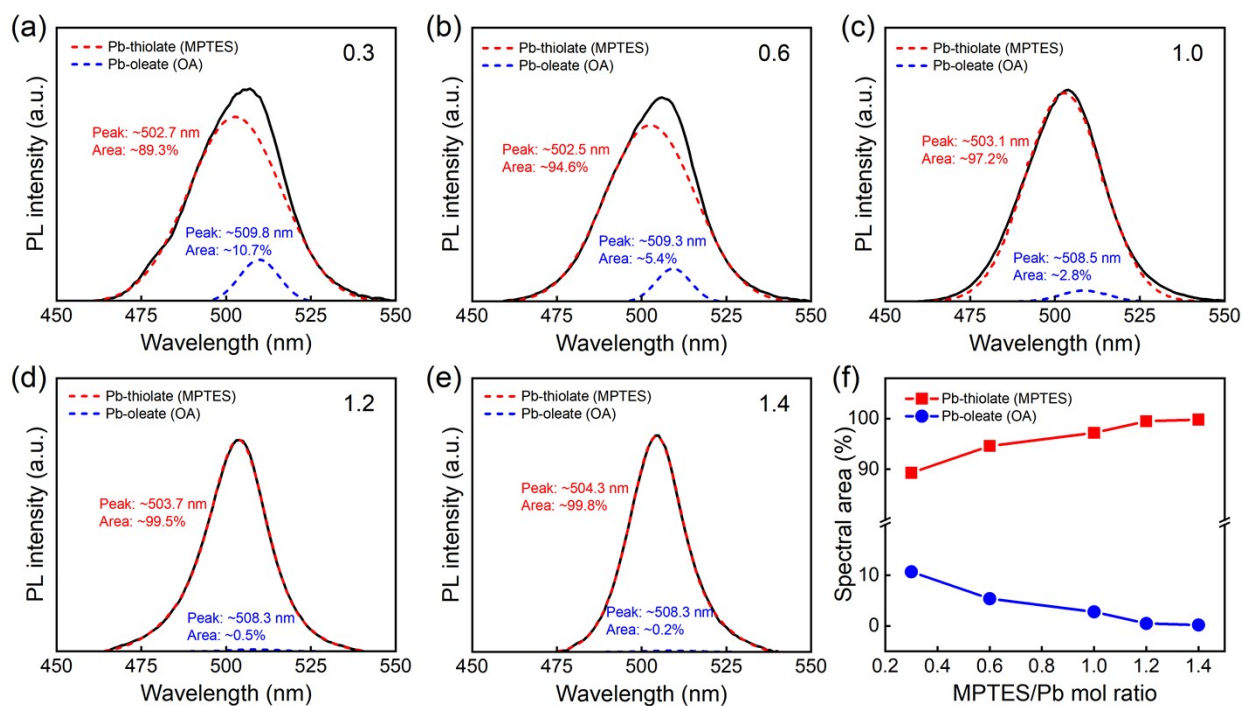


Figure S2. (a-e) Deconvoluted PL spectra of core-shell M-CsPbBr₃ QDs fabricated as a function of MPTES concertation (MPTES/Pb mol ratio). (f) Contribution of each CsPbBr₃ QDs (pristine CsPbBr₃ QDs and core-shell M-CsPbBr₃ QDs) fabricated from Pb-olate (OA) and Pb-thiolate (MPTES) to PL intensity. MPTES was injected into the Pb-pot immediately after degassing the Pb-pot. Reaction time was ~5 s.

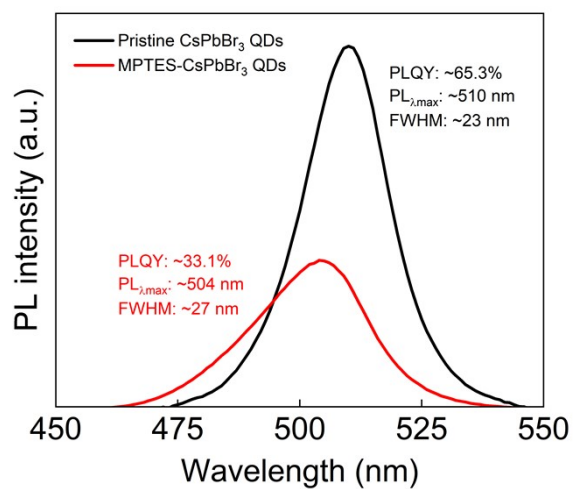


Figure S3. PL spectra of pristine CsPbBr₃ QDs and MPTES-CsPbBr₃ QDs. MPTES-CsPbBr₃ QDs were fabricated by substituting OA with MPTES (OA-free) as a ligand (see Experimental method). MPTES (MPTES/Pb mol ratio of 1.0) was injected into the Pb-pot immediately after degassing the Pb-pot. Reaction time was ~5 s.

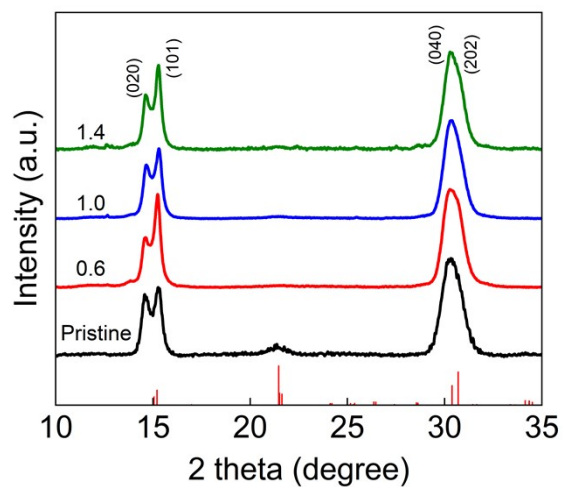


Figure S4. XRD patterns of pristine CsPbBr₃ QDs and core-shell M-CsPbBr₃ QDs as a function of MPTES concentration (MPTES/Pb mol ratio). The pristine CsPbBr₃ QDs and core-shell M-CsPbBr₃ QDs showed the orthorhombic crystal structure (JCPDS card no. 98-009-7851). MPTES was injected into the Pb-pot immediately after degassing the Pb-pot. Reaction time was ~5 s.

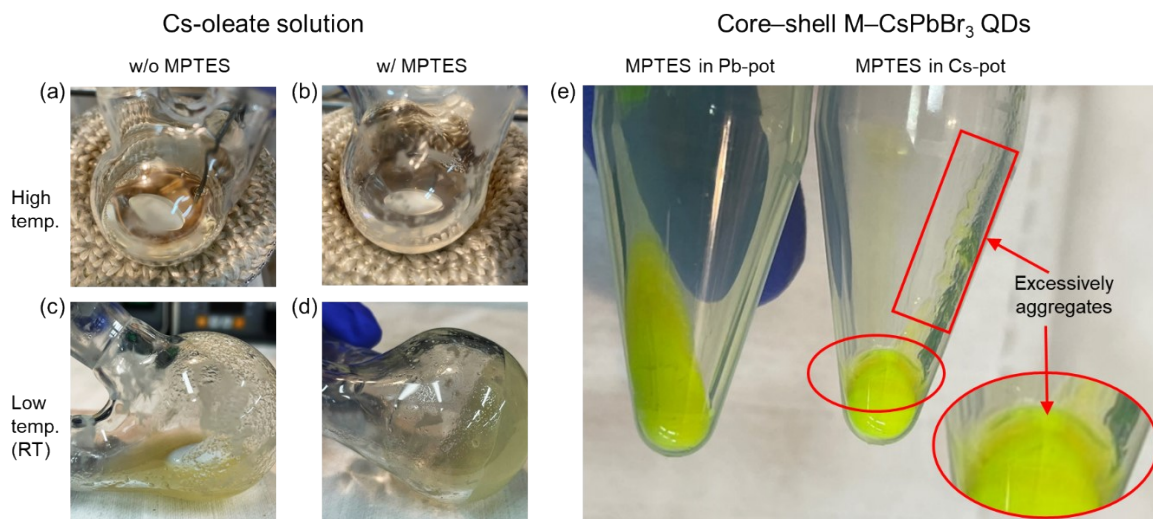


Figure S5. Digital photograph of **(a, c)** Cs-oleate solution and **(b, d)** Pre-mixed solution (Cs-oleate with MP TES). **(e)** Digital photograph of precipitated core-shell M-CsPbBr₃ QDs after purification. **(e, left)** The core-shell M-CsPbBr₃ QDs were fabricated using Cs-oleate solution. **(e, right)** core-shell M-CsPbBr₃ QDs was fabricated using pre-mixed (MP TES and Cs-oleate) solution.

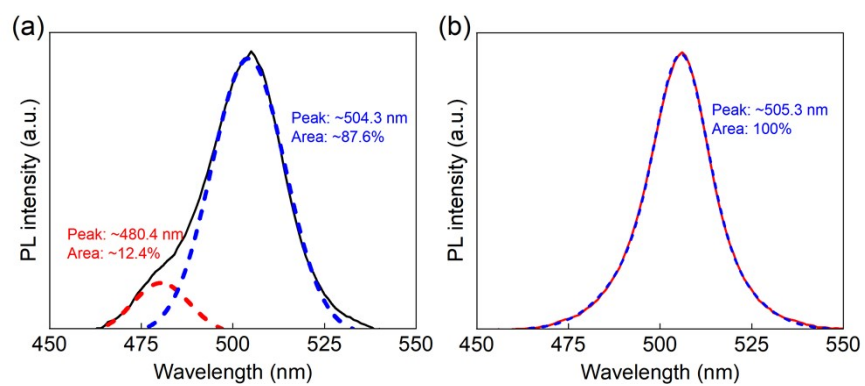


Figure S6. Deconvoluted PL spectra of core-shell M-CsPbBr₃ QDs fabricated under different reaction time. **(a)** ~5 s and **(b)** ~20 s. MPTES (MPTES/Pb mol ratio of 1.4) was injected into the Pb-pot immediately before Cs-oleate injection.

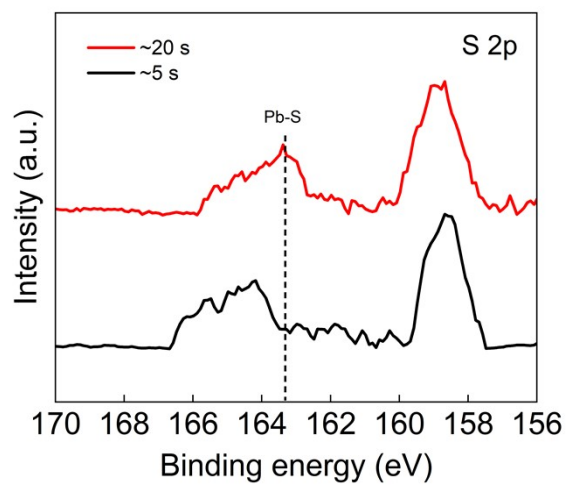


Figure S7. XPS spectra of core-shell M-CsPbBr₃ QDs fabricated under different reaction times. MPTES (MPTES/Pb mol ratio of 1.4) was injected into the Pb-pot immediately before Cs-oleate injection.

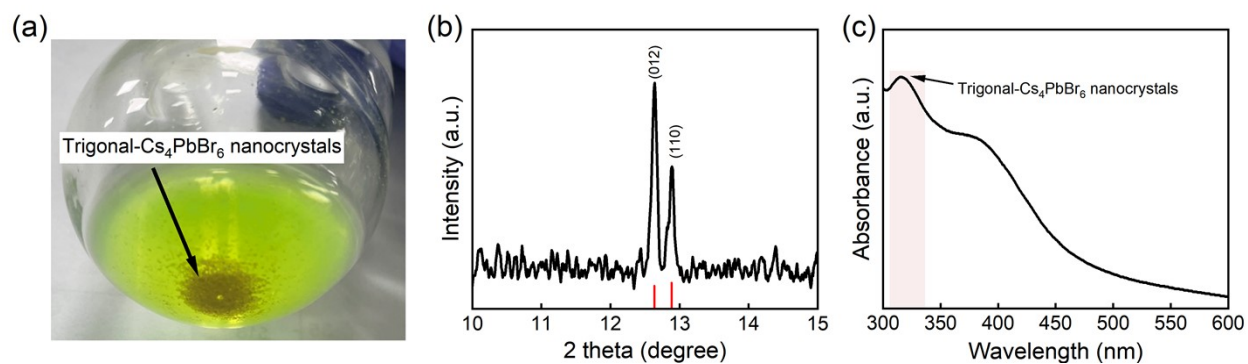


Figure S8. (a) Digital photograph of trigonal-Cs₄PbBr₆ nanocrystals precipitated in crude solution. (b) XRD pattern, and (c) absorbance spectrum of trigonal-Cs₄PbBr₆ nanocrystals. MPTES was injected into the Pb-pot immediately before Cs-oleate injection. MPTES/Pb mol ratio was 3.0 and reaction time was ~20s.

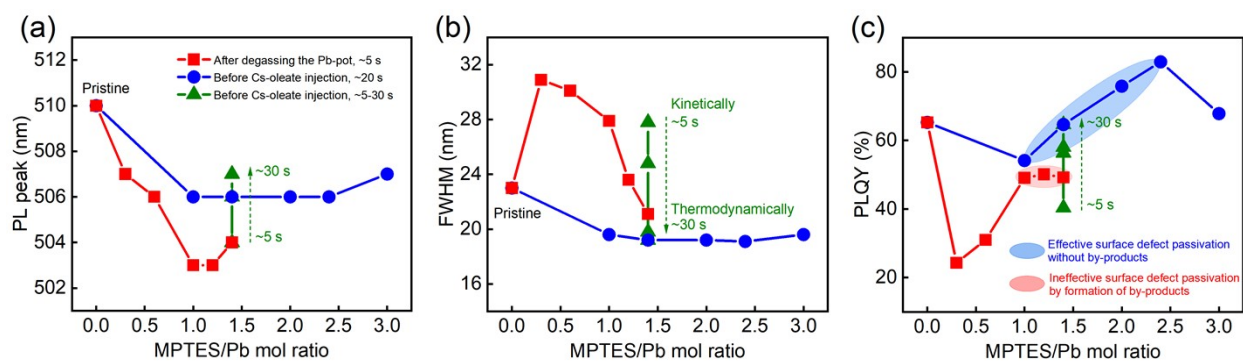


Figure S9. Effect of synthetic parameters (MP TES injection time, MP TES concentration (MP TES/Pb mol ratio), and reaction time) on the optical properties of core-shell M-CsPbBr₃ QDs. **(a)** PL_{λ_{max}}, **(b)** FWHM, and **(c)** PLQYs.

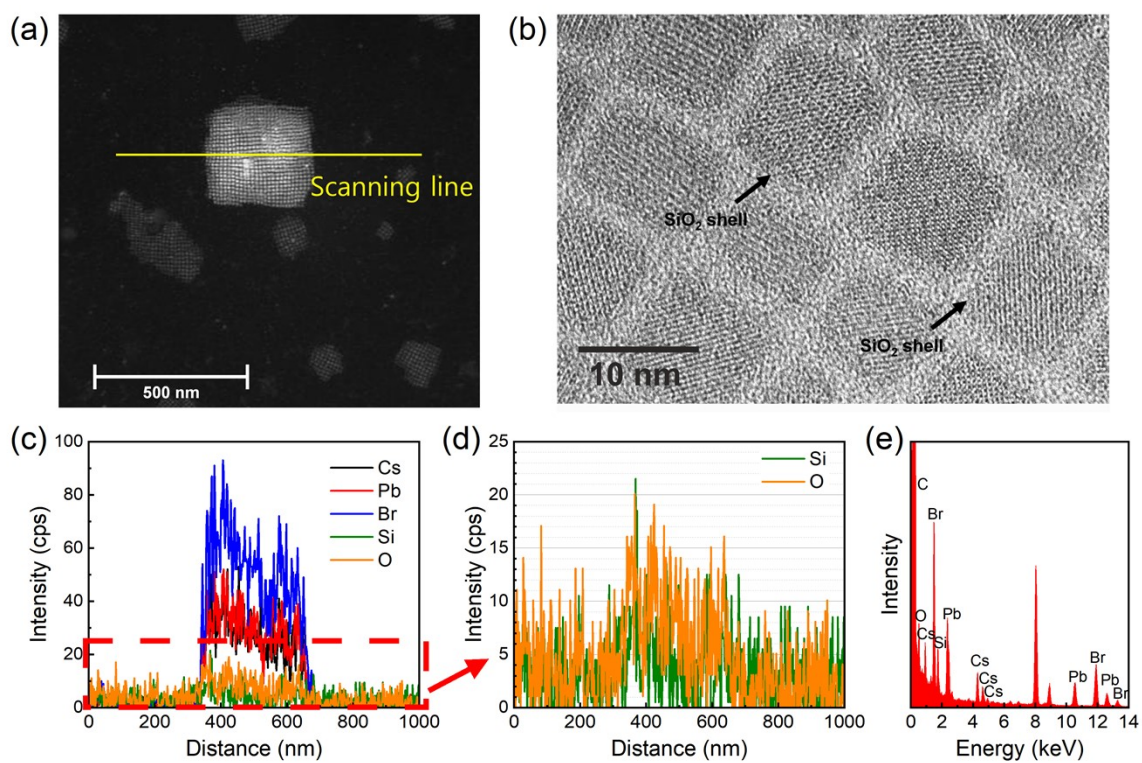


Figure S10. (a) Scanning transmission electron microscopy (STEM) image of core-shell M-CsPbBr₃ QDs cluster. (b) High magnified HR-TEM image of core-shell M-CsPbBr₃ QDs. (c-e) TEM-EDS line scanning profiles and spectrum.

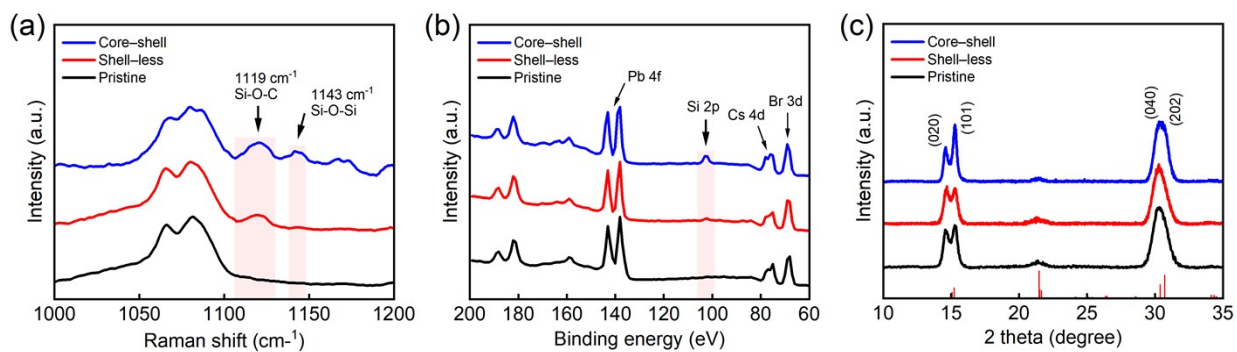


Figure S11. (a) Raman spectra, (b) XPS spectra and (c) XRD patterns of pristine CsPbBr_3 QDs, shell-less M- CsPbBr_3 QDs and core-shell M- CsPbBr_3 QDs. MPTES was injected into the Pb-pot immediately before Cs-oleate injection. MPTES/Pb mol ratio was 2.4 and reaction time was ~ 20 s.

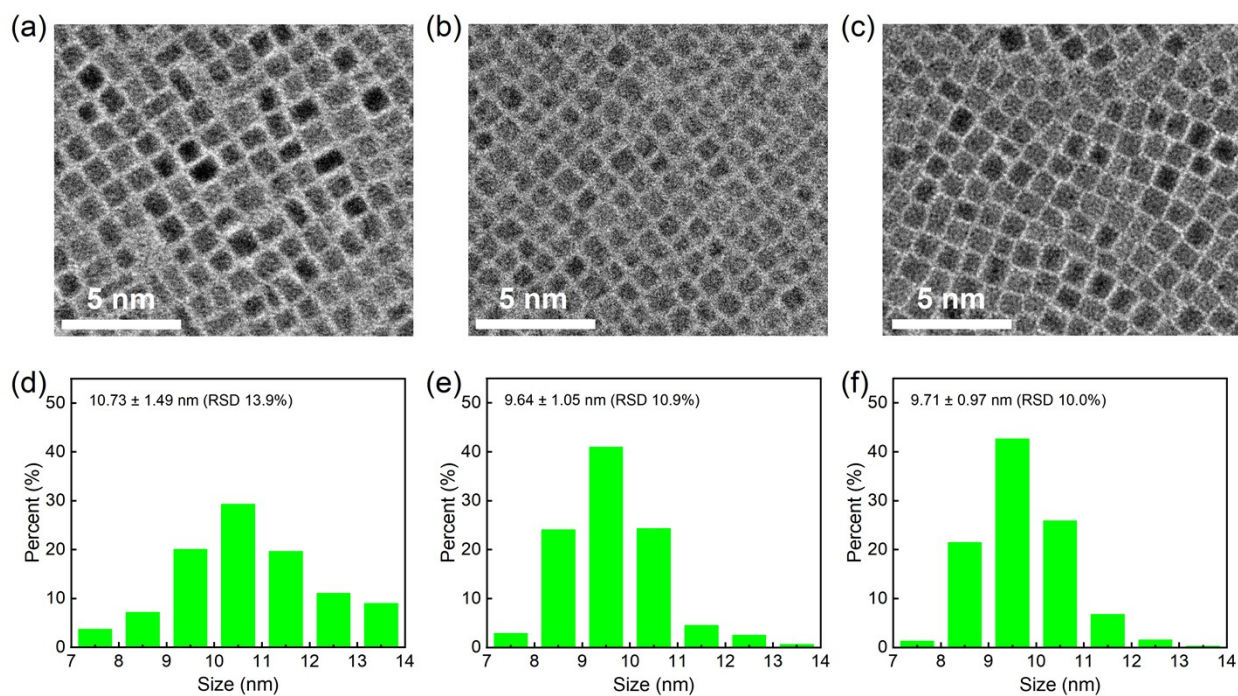


Figure S12. HR-TEM images and size distributions of three CsPbBr₃ QDs. **(a)** and **(d)** pristine CsPbBr₃ QDs, **(b)** and **(e)** shell-less M-CsPbBr₃ QDs, **(c)** and **(f)** core-shell M-CsPbBr₃ QDs. MPTES was injected into the Pb-pot immediately before Cs-oleate injection. MPTES/Pb mol ratio was 2.4 and reaction time was ~20 s.

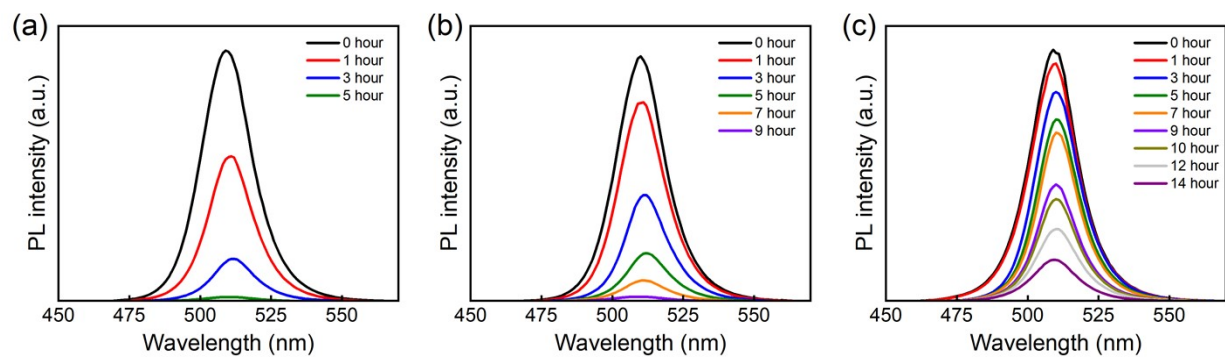


Figure S13. The PL spectra of (a) pristine CsPbBr₃ QDs, (b) shell-less M-CsPbBr₃ QDs, and (c) core-shell M CsPbBr₃ QDs as a function of immersion time in DI water.

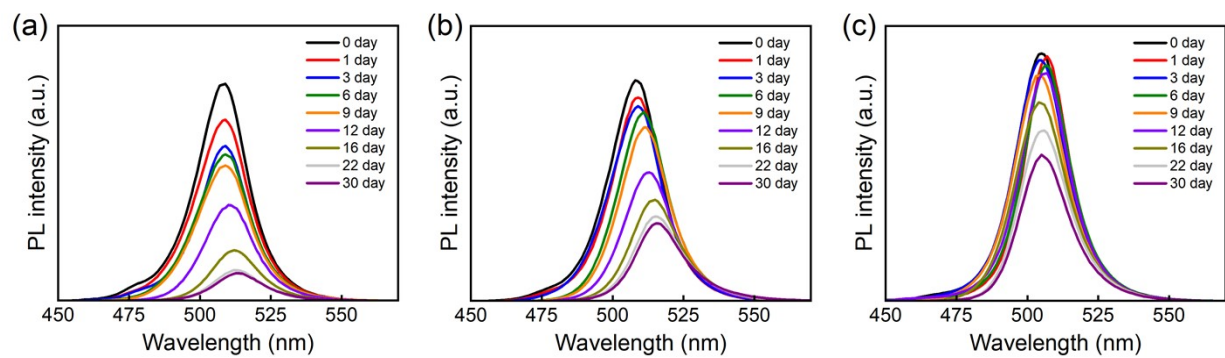


Figure S14. The PL spectra of (a) pristine CsPbBr₃ QDs, (b) shell-less M-CsPbBr₃ QDs, and (c) core-shell M-CsPbBr₃ QDs as a function of air exposure time.

Table S1. Element quantitative analysis result of core-shell M-CsPbBr₃ QDs

Element	Weight %	Atomic %
Cs	25.70	17.27
Pb	30.75	13.25
Br	37.14	41.49
Si	3.24	10.30
O	3.17	17.69

Movie S1. Color change of the Pb-pot after MPTES injection (MPTES/Pb mol ratio of 0.6). MPTES was injected into the Pb-pot immediately after degassing the Pb-pot. (8x speed).

Movie S2. Color change of the Pb-pot after MPTES injection (MPTES/Pb mol ratio of 1.4). MPTES was injected into the Pb-pot immediately after degassing the Pb-pot. (8x speed).

Movie S3. Color change of the Pb-pot after MPTES injection (MPTES/Pb mol ratio of 2.4). MPTES was injected into the Pb-pot immediately before Cs-oleate injection.