Supporting Information

Broad Band and Massive Stokes Shift Luminescence in Fully Inorganic 2D Layered Perovskite $CsPb_2Cl_5$: Single Crystal Growth and Self-Trapped Exciton Emission

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1. Descriptions of the raw materials purity and crystal growth process

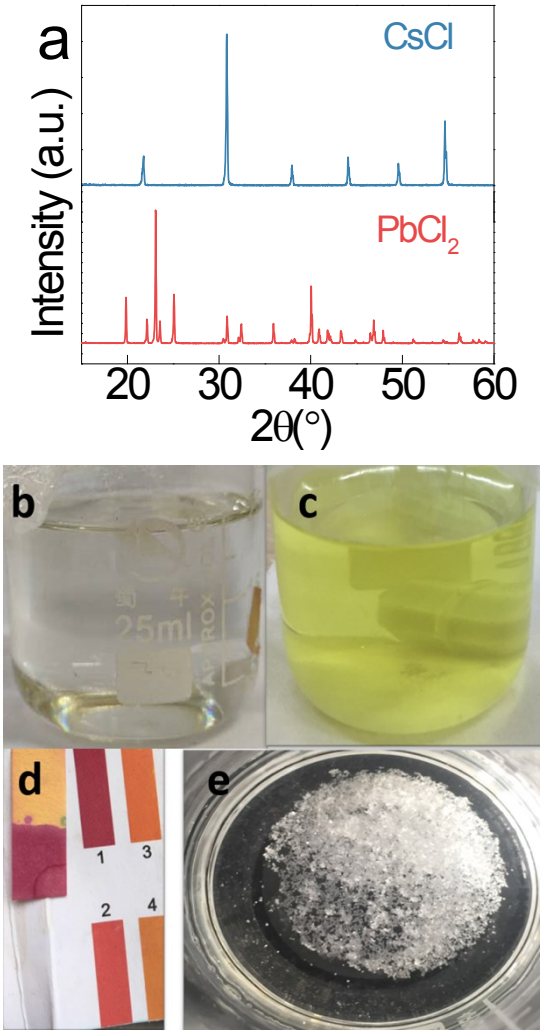

Figure S1. (a) XRD patterns of CsCl and $PbCl_2$; (b) The solution dissolved CsCl and $PbCl_2$; (c) Light yellow solution after growing for a period; (d) The pH value of the solution; (e) Large number of spontaneous small opaque crystals.

2. Pure $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ single crystals

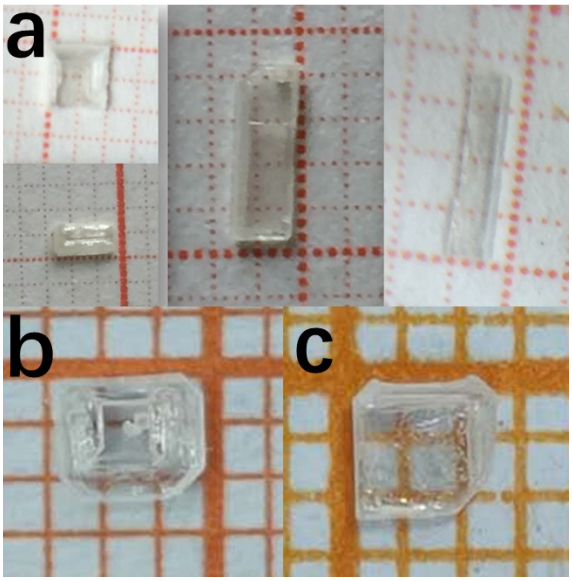

Figure S2. (a-b) Photos of pure $CsPb_2Cl_5$ SCs grown with the molar ratio of CsCl to $PbCl_2$ of 1:1 and 1:2 respectively; (c) Photo of $CsPb_2(Cl_{0.95}Br_{0.05})_5$ SC.

3. (002) planes XRD patterns of $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ SCs

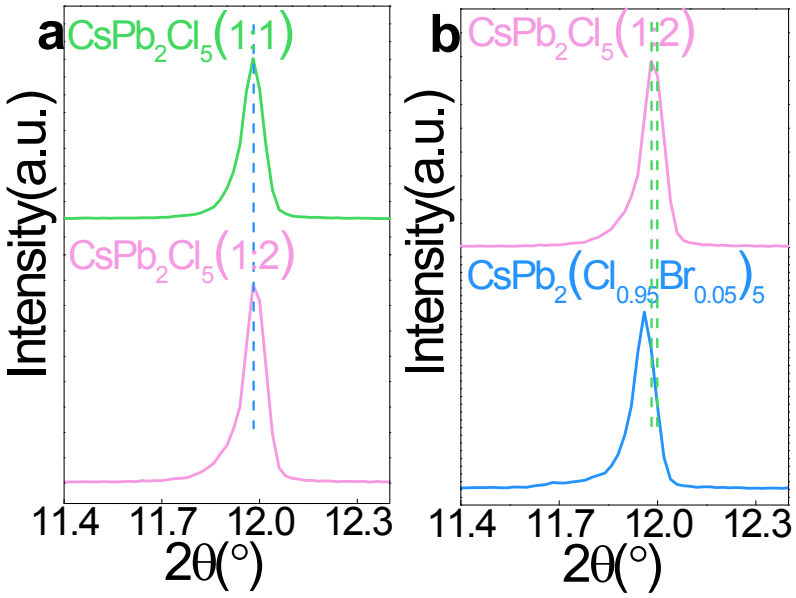

Figure S3. (a-b) Magnified XRD of pure $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ for (002) plane.

4. The bond lengths and bond angles of $[Pb\text{-}Cl]_8$ and $[Cs\text{-}Cl]_{10}$ polyhedrons

Table S1. List of Pb-Cl and Cs-Cl bond lengths in $[Pb\text{-}Cl]_8$ and $[Cs\text{-}Cl]_{10}$ polyhedrons.

Atoms	Pb			Cs	
Neighbor Cl	2 Cl_1	2 Cl_2	4 Cl_3	2 Cl_4	8 Cl_5
Distance (Å)	2.753(8)	3.024(7)	3.210(3)	3.693(2)	3.589(6)

Table S2. List of bond angles between neighbor $[Pb\text{-}Cl]_8$ and $[Cs\text{-}Cl]_{10}$ polyhedrons.

Atoms1-2-3	Angle1-2-3 (°)	Atoms1-2-3	Angle1-2-3 (°)
Cl_1-Pb-Cl_1	84.306(57)	Cl_4-Cs-Cl_4	180.000
Cl_1-Pb-Cl_2	76.687(36)	Cl_4-Cs-Cl_5	59.068(44)
Cl_2-Pb-Cl_2	143.809(22)	Cl_4-Cs-Cl_5	120.932(47)
Cl_1-Pb-Cl_3	93.477(51)	Cl_5-Cs-Cl_5	74.679(41)
Cl_1-Pb-Cl_3	146.455(56)	Cl_5-Cs-Cl_5	118.136(37)
Cl_2-Pb-Cl_3	70.263(32)	Cl_5-Cs-Cl_5	73.558(58)
Cl_2-Pb-Cl_3	135.419(34)	Cl_5-Cs-Cl_5	76.845(39)
Cl_3-Pb-Cl_3	67.050(48)	Cl_5-Cs-Cl_5	139.116(42)
Cl_3-Pb-Cl_3	70.296(44)	Cl_5-Cs-Cl_5	144.241(42)
Cl_3-Pb-Cl_3	105.837(50)	Cs-Cl_4-Cs	57.288(13)
Pb-Cl_1-Pb	91.324(45)	Cs-Cl_5-Cs	106.442(41)
Pb-Cl_2-Pb	90.000	-----	-----
Pb-Cl_3-Pb	74.163(36)	-----	-----

5. Full XPS profiles of $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ SCs

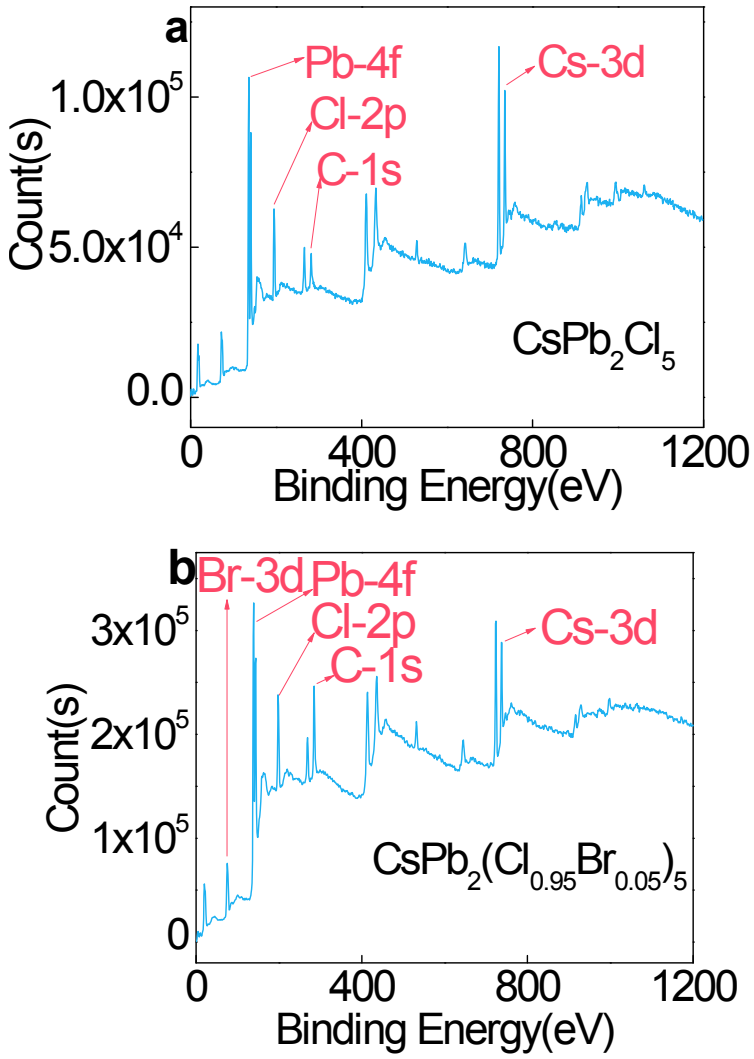

Figure S4. (a-b) Full XPS profiles of $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ SCs.

6. XPS binding energy of $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ SCs

Table S3. Comparison of XPS binding energy of $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ SCs.

Samples / Elements	Binding Energy(eV)	
	$CsPb_2Cl_5$	$CsPb_2(Cl_{0.95}Br_{0.05})_5$
Cs-3d	723.8	723.5
	737.8	737.5
Pb-4f	138.6	138.7
	143.5	143.5
Cl-2p	197.9	197.9
	199.5	199.4
Br-3d	----	67.9
	----	67.0

7. The PL spectra of different references, $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ powders

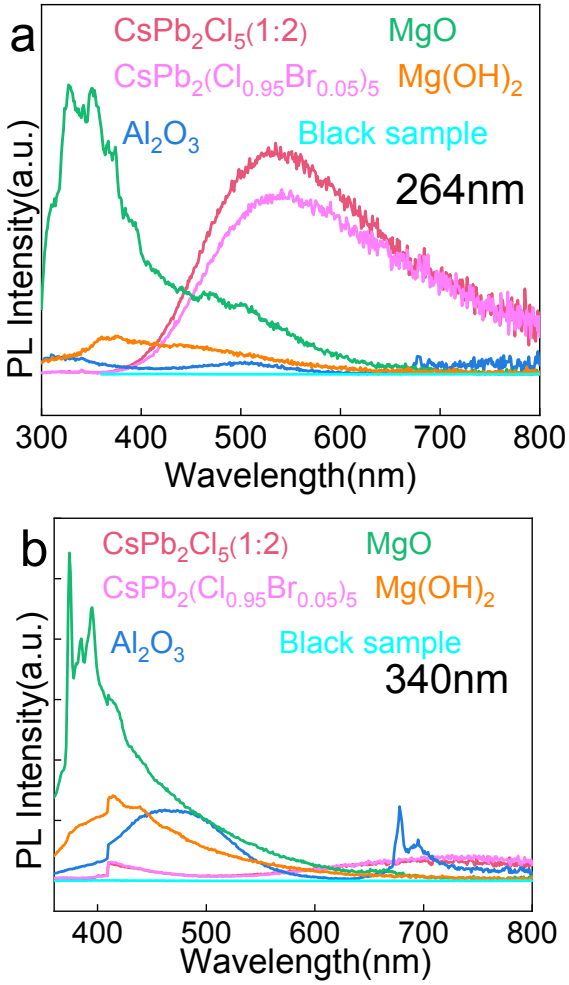

Figure S5. (a-b) The PL spectra of different reference substances, $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ crystal.

8. Photoluminescence spectra of $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ SCs obtained at various excitation energy densities

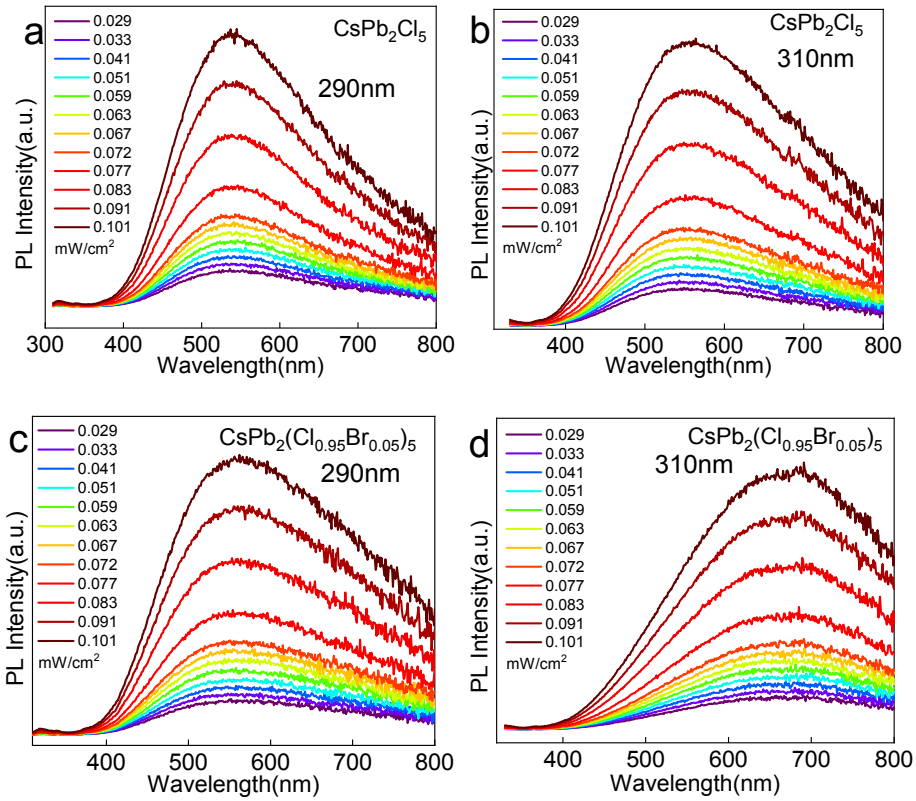

Figure S6. (a-d) Photoluminescence spectra of $CsPb_2Cl_5$ and $CsPb_2(Cl_{0.95}Br_{0.05})_5$ SCs obtained at various excitation energy densities under the excitation of 290 and 310 nm.

9. The XRD of initial $CsPb_2Cl_5$ and after soaking for 2 hours using a 306 nm illumination.

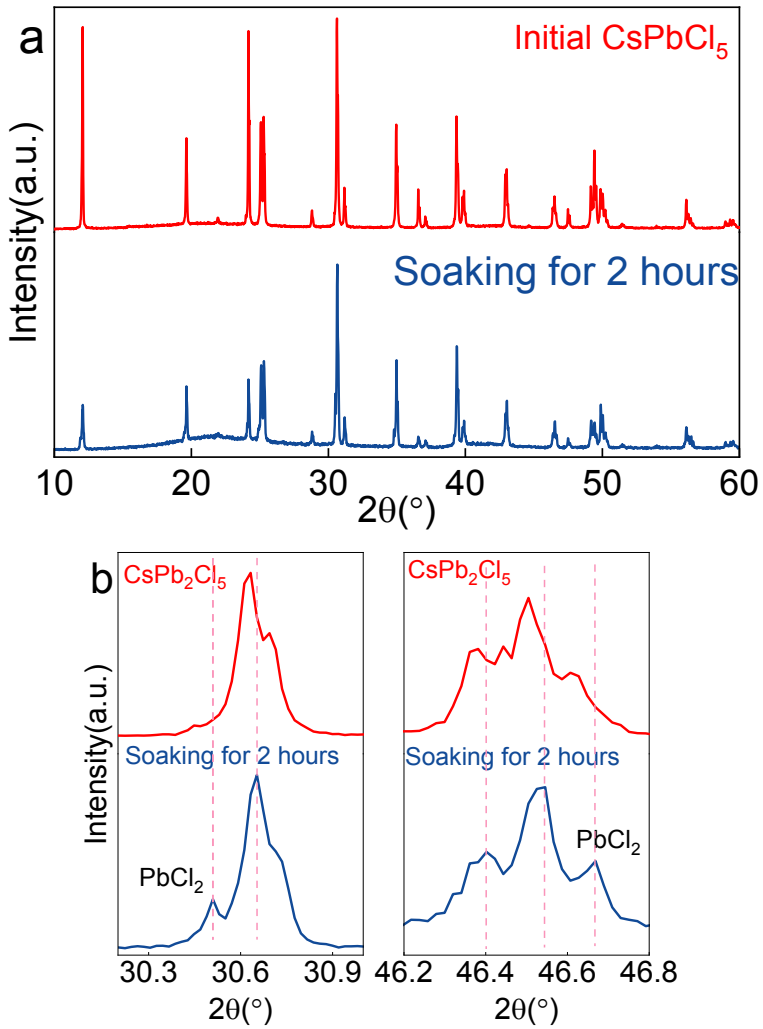

Figure S7. (a-b) The XRD and Magnified XRD of initial $CsPb_2Cl_5$ and after soaking for 2 hours using a 306 nm illumination.