Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting information

Tunable optical property and stability of lead free all inorganic perovskite ($Cs_2SnI_{6-x}Cl_x$)

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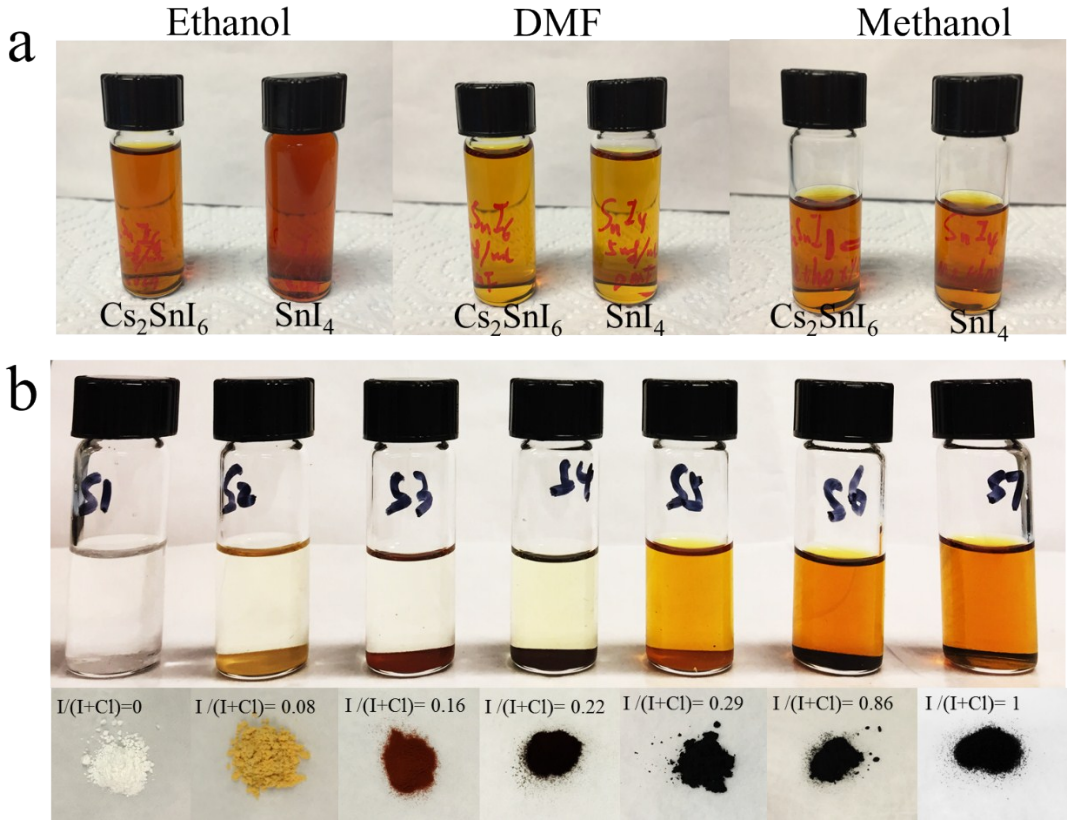

Fig. S1 (a) Cs_2SnI_6 and SnI_4 were dissolved in ethanol, Dimethylformamide (DMF) and methanol, respectively. (b) $Cs_2SnI_xCl_{6-x}$ perovskite in ethanol solution. The corresponding powder is shown under each vial. The concentration is 5 mg/mL.

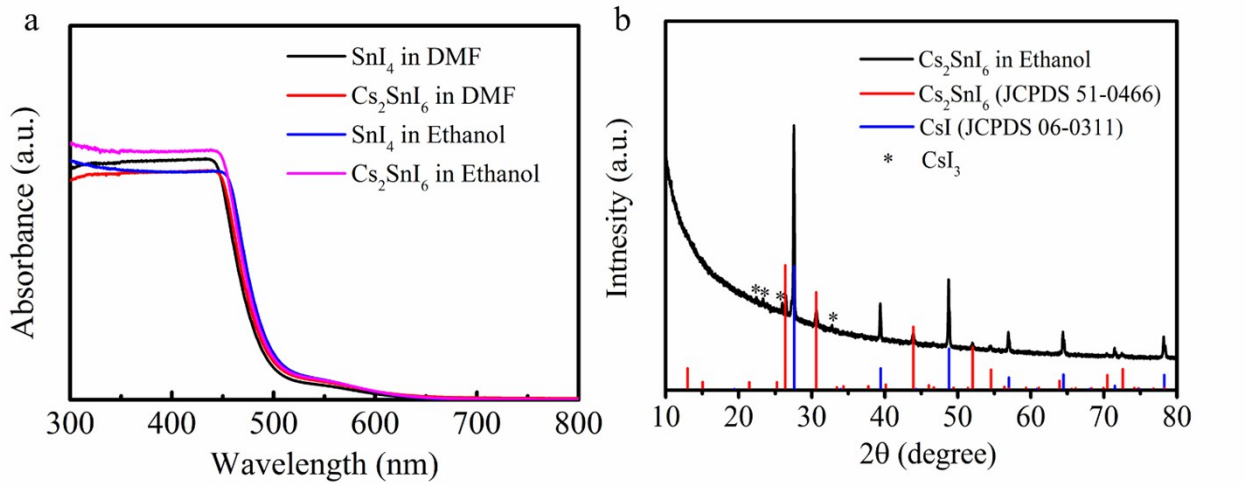

Fig. S2 (a) UV-vis absorption spectra of Cs_2SnI_6 and SnI_4 in DMF and Ethanol solution, respectively. (b) XRD pattern of Cs_2SnI_6 in Ethanol solution dried at 60 °C.

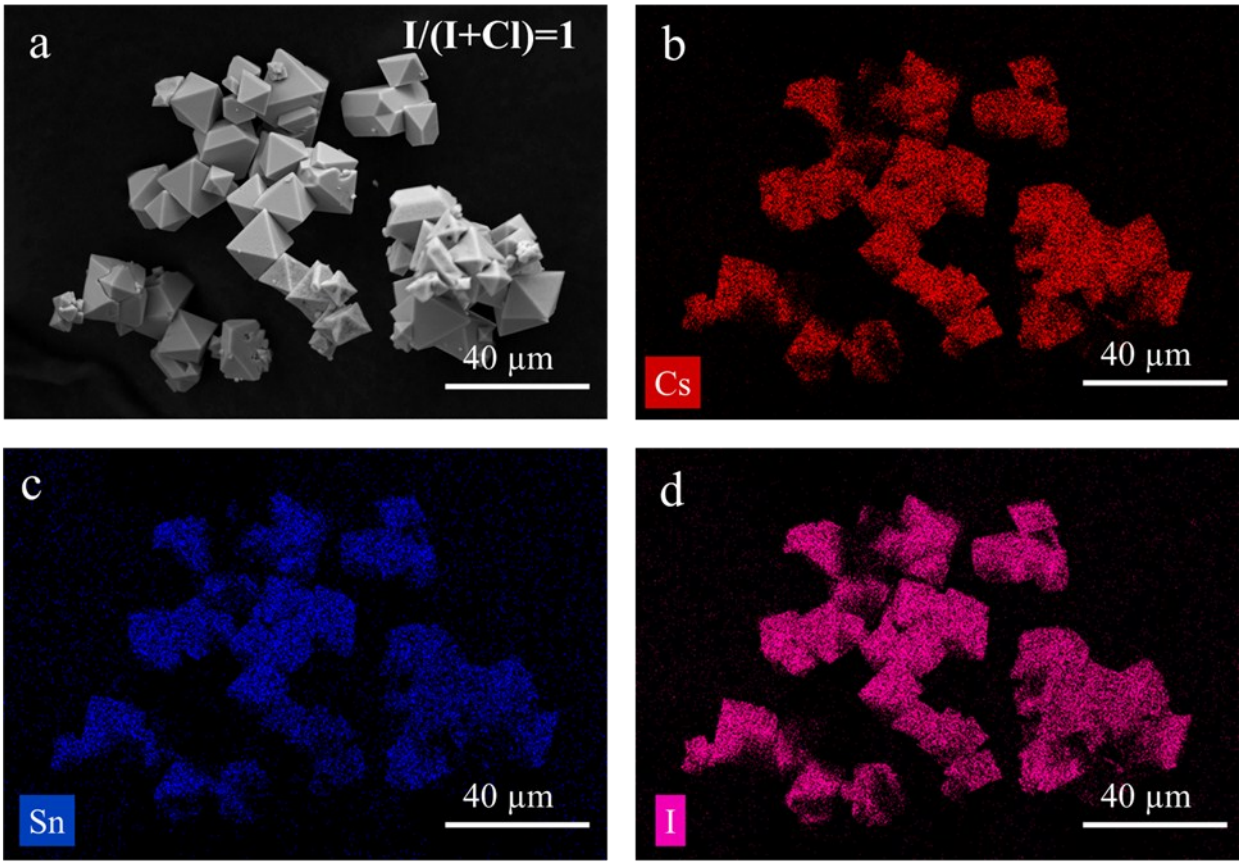

Fig. S3 (a) SEM image of the sample S7 (Cs_2SnI_6), (b) Cs map, (c) Sn map, (d) I map.

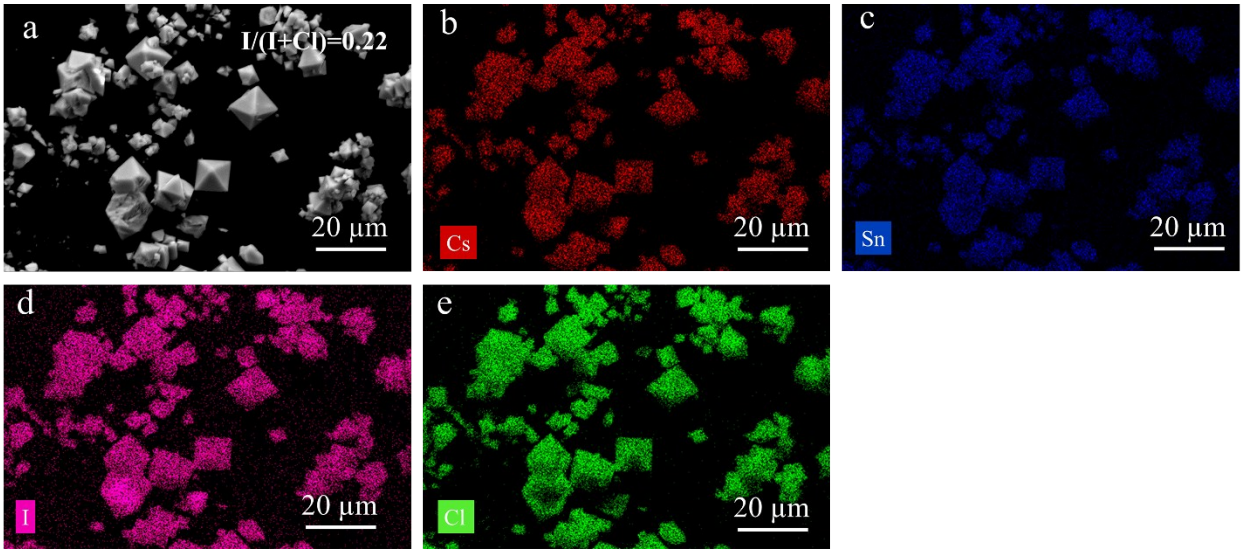

Fig. S4 (a) SEM image of the sample S4, (b-e) the corresponding elemental mappings of Cs, Sn, I and Cl, respectively.

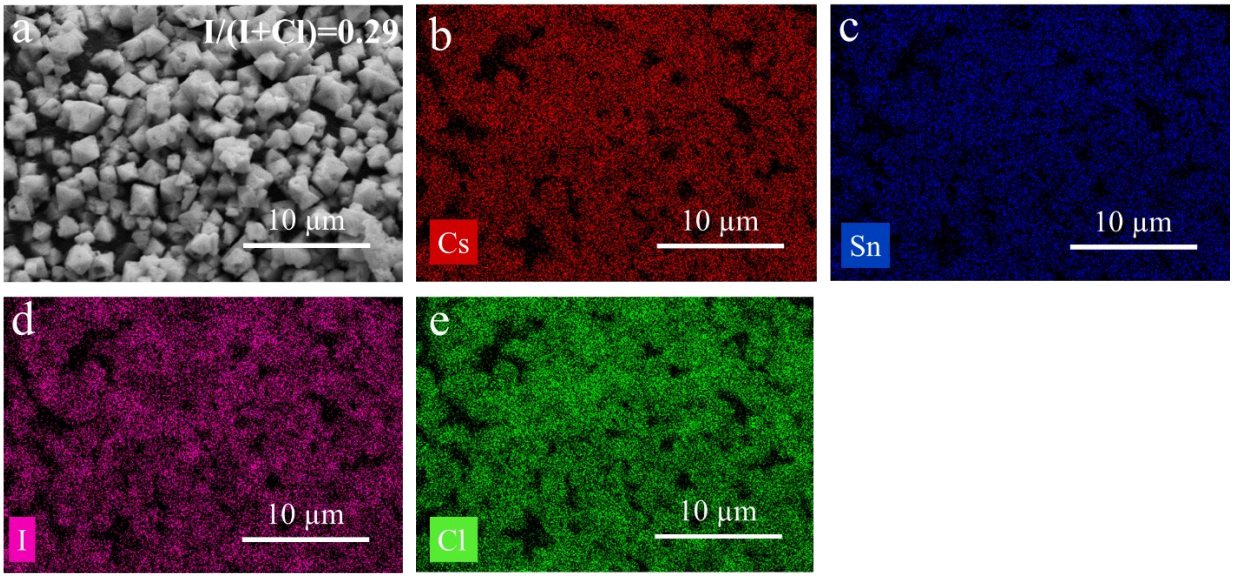

Fig. S5 (a) SEM image of sample S5, (b-e) the corresponding elemental mapping of Cs, Sn, I and Cl, respectively.

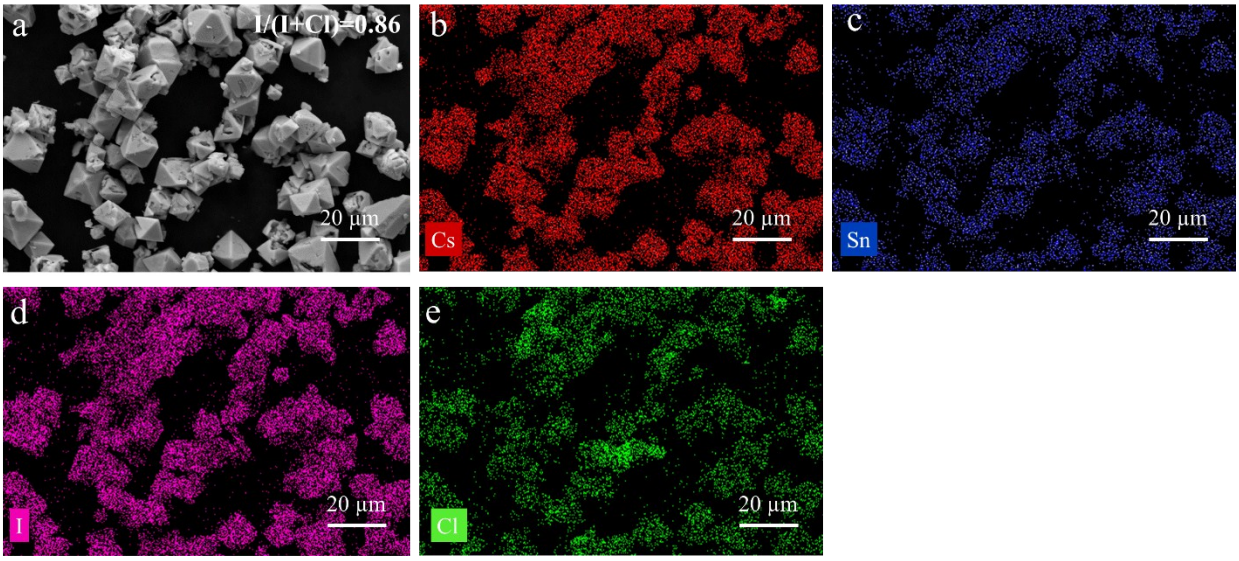

Fig. S6 (a) SEM image of sample S6, (b-e) the corresponding elemental mapping of Cs, Sn, I and Cl, respectively.

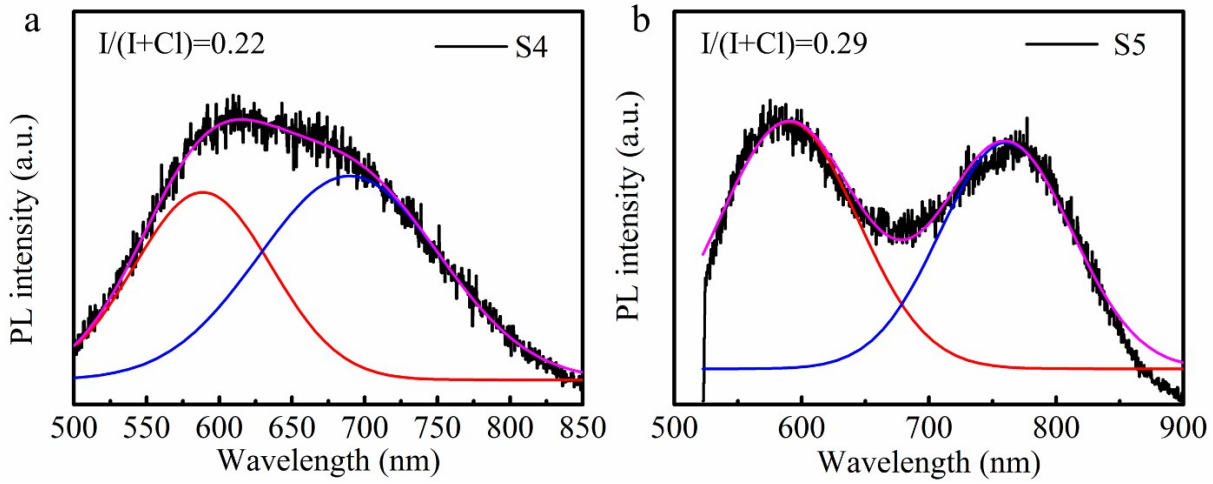

Fig. S7 Multi-peak fitting of PL spectra at room temperature for sample (a) S4 and (b) S5. The bandgaps of these peaks are identified for S4 (2.11 eV and 1.82 eV) and S5 (2.08 eV and 1.63 eV), respectively.

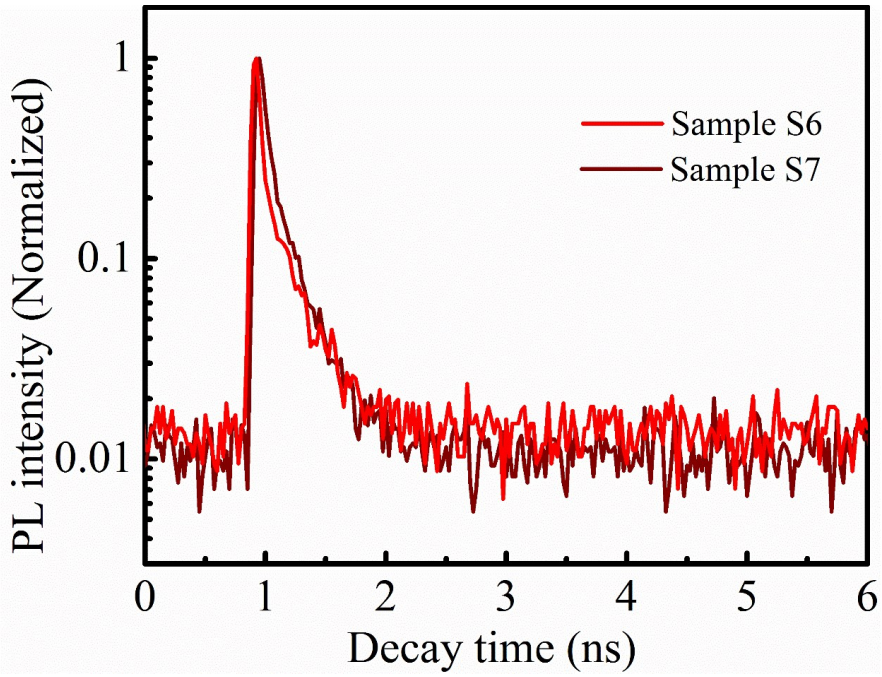

Fig. S8 Time-resolved photoluminescence measured at room temperature for sample S6 ($Cs_2SnI_{5.28}Cl_{0.72}$) and S7 (Cs_2SnI_6).

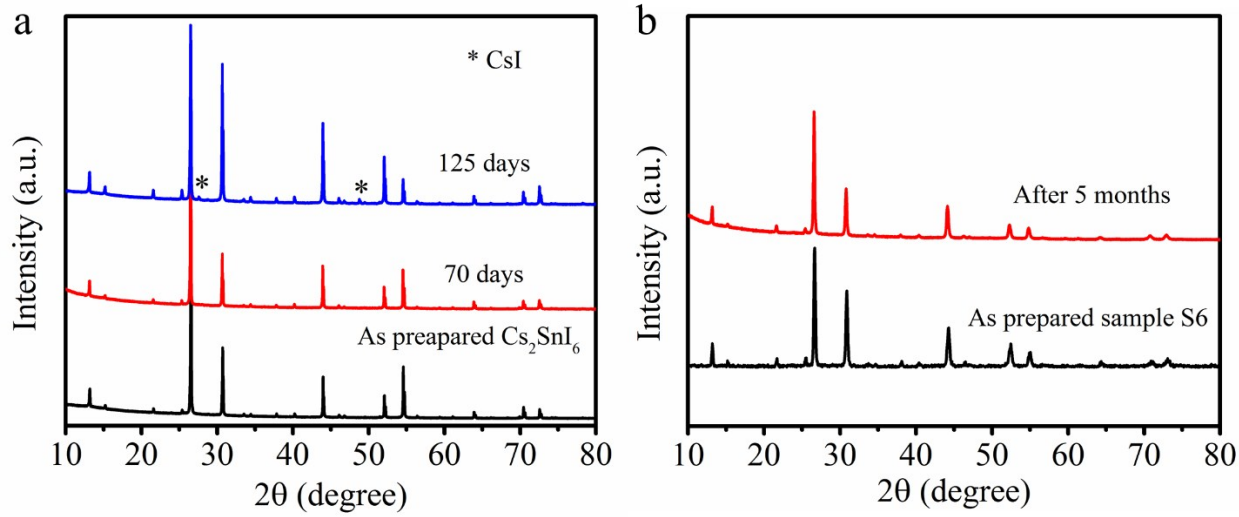

Fig. S9 (a) XRD patterns of the sample S7 (Cs_2SnI_6) stored at ambient condition for 0, 70 and 125 days, (b) XRD patterns of the sample S6 ($Cs_2SnI_{5.28}Cl_{0.72}$) stored at ambient condition for 0 day and 5 months.

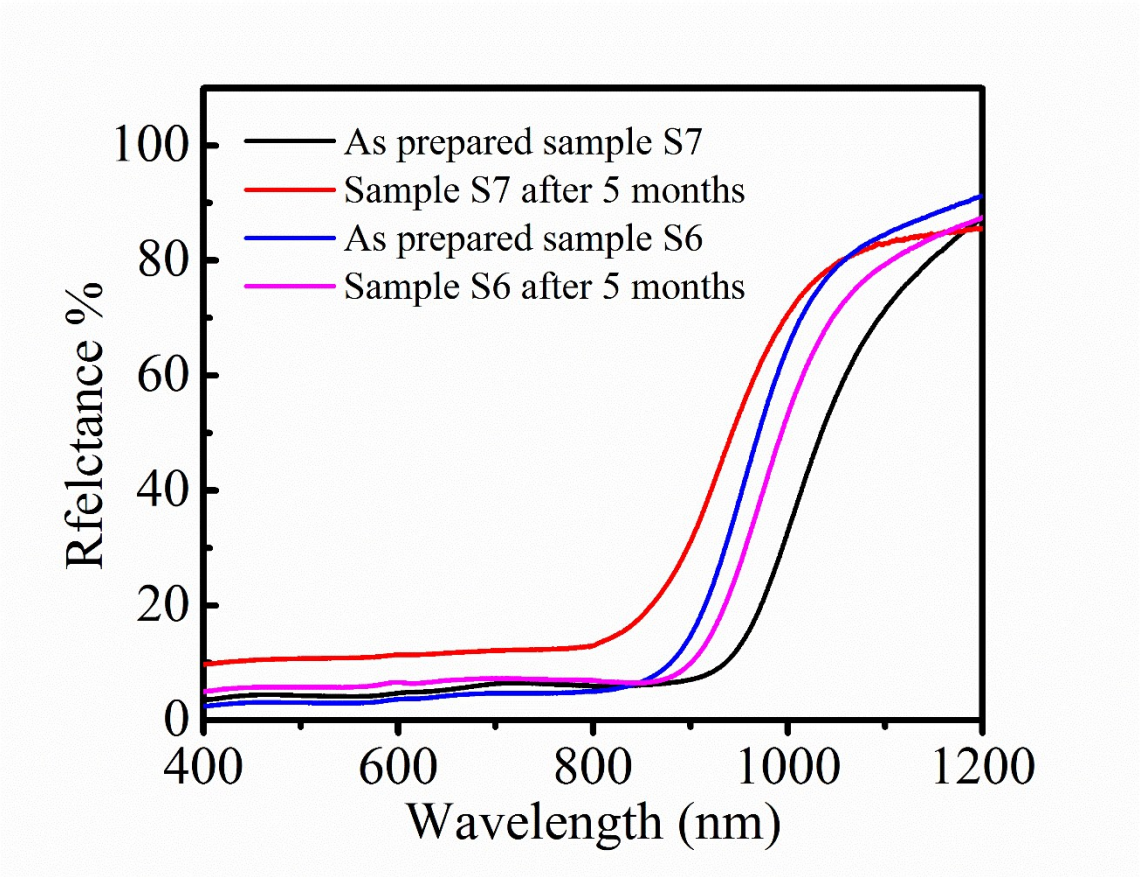

Fig. S10 UV-vis diffuse reflectance spectra of sample S7 (Cs_2SnI_6) and S6 ($Cs_2SnI_{5.28}Cl_{0.72}$) as prepared and after 5 months, respectively.

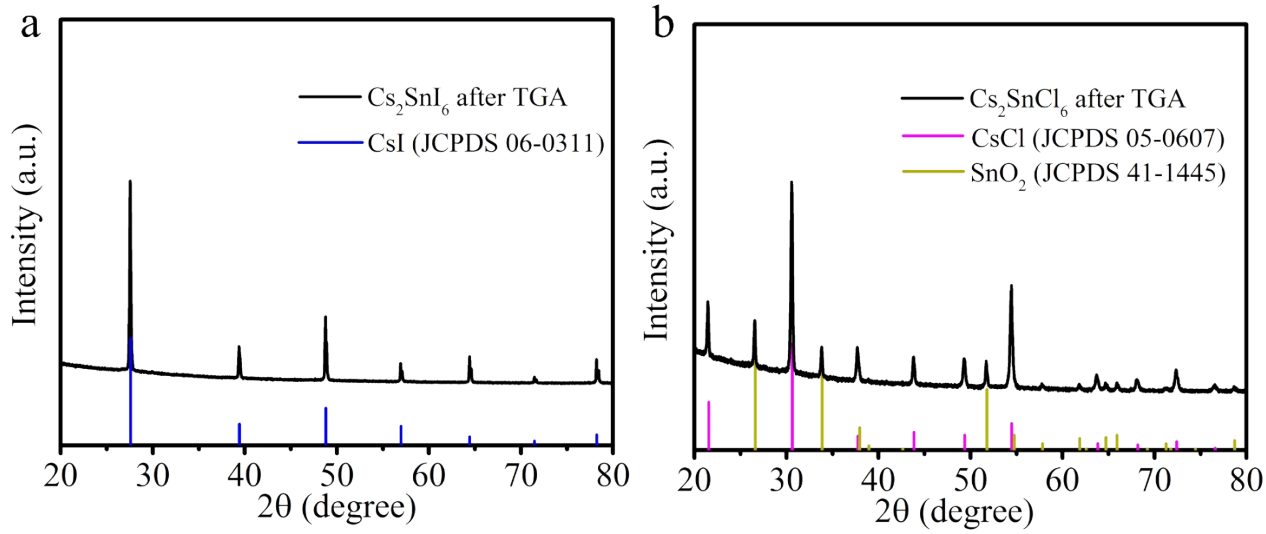

Fig. S11 (a) the XRD patterns for Cs_2SnI_6 sample after TGA measurement. All peaks can be matched to the standard file JCPDS 06-0311of CsI. (b) the XRD pattern for the residual of Cs_2SnCl_6 sample after TGA test. All peaks can be matched to the standard files of CsCl (JCPDS 05-0607) and SnO_2 (JCPDS 41-1445).

Table S1 Structure parameters and refinement statistics for $Cs_2SnI_xCl_{6-x}$ from Rietveld refinement of synchrotron X-ray powder diffraction data

Sample	S1	S2	S3	S4			S5		S6	S7
stoichiometric x	0	0.43	0.90	0.69	1.3	5.21	0.44	5.36	5.28	6
a (Å)	10.3923 (2)	10.5561(2)	10.6741(1)	10.6310(5)	10.7620(5)	11.5503 (23)	10.5255(4)	11.6097(3)	11.5870(2)	11.6517(2)
Phase fraction (%)	100	100	100	48.9	49.5	1.6	61.1	38.9	100	100
Cl/I (x, 0, 0)	0.2320(2)	0.2368(2)	0.2406(2)	0.2404(4)	0.2407(4)	0.2378(39)	0.2384(4)	0.2462(3)	0.2450(2)	0.2450(1)
U_{iso} (Cs) (Å^2)	0.0275(9)	0.0532(7)	0.0663(8)	0.0485(14)	0.0846(22)	0.076(48)	0.0451(15)	0.0557(32)	0.0546(17)	0.0240(13)
U_{iso} (Sn) (Å^2)	0.0414(7)	0.0365(9)	0.0435(9)	0.0316(17)	0.0477(23)	0.047(40)	0.0319(19)	0.0338(30)	0.0324(18)	0.0423(10)
U_{iso} (Cl/I) (Å^2)	0.0451(11)	0.0527(14)	0.0623(12)	0.0484(21)	0.0651(24)	0.093(25)	0.0498(26)	0.0393(13)	0.0395(7)	0.0351(5)
RF^2 (%)	4.23	3.86	5.65	4.42	3.93	8.36	3.42	2.96	5.27	5.24
R_{wp} (%)	4.39	4.63	4.68		3.88		5.70		7.90	6.62
GOF	4.33	4.05	4.61		3.62		5.48		7.31	5.68

Note. Sample S4 has three phases, two major phases with close compositions and a third I-rich phase.
Sample S5 has two phases with I- and Cl-enriched compositions.