

Supporting Information for:

Highly efficient and stable broadband near-infrared-emitting lead-free metal halide double perovskites

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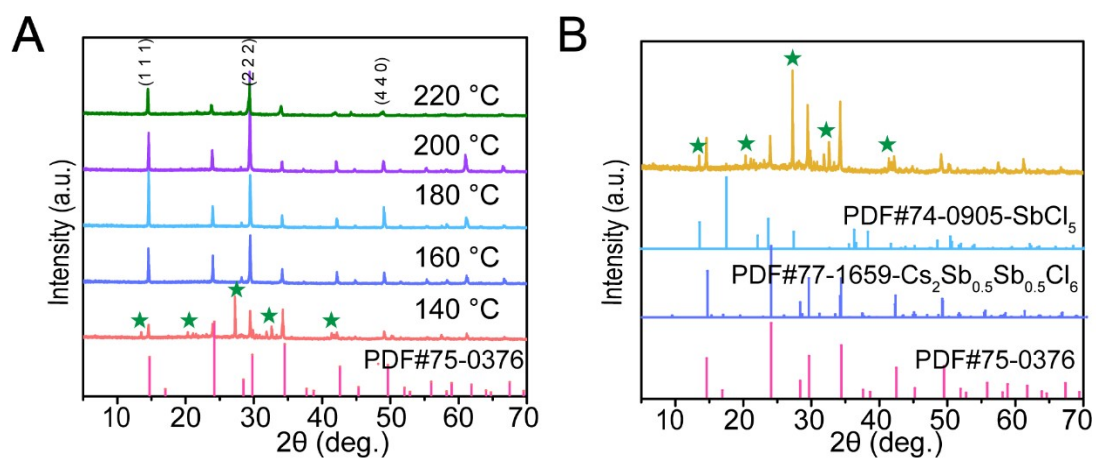


Fig. S1. A) XRD patterns $\text{Cs}_2\text{SnCl}_4\text{Br}_2:0.02\text{Sb}$ prepared at different synthesis temperatures and the standard XRD pattern of Cs_2SnCl_6 . B) XRD patterns $\text{Cs}_2\text{SnCl}_4\text{Br}_2:0.02\text{Sb}$ prepared at 140 °C and the standard XRD patterns of $\text{Cs}_2\text{Sb}_{0.5}\text{Sb}_{0.5}\text{Cl}_6$ and SbCl_5 .

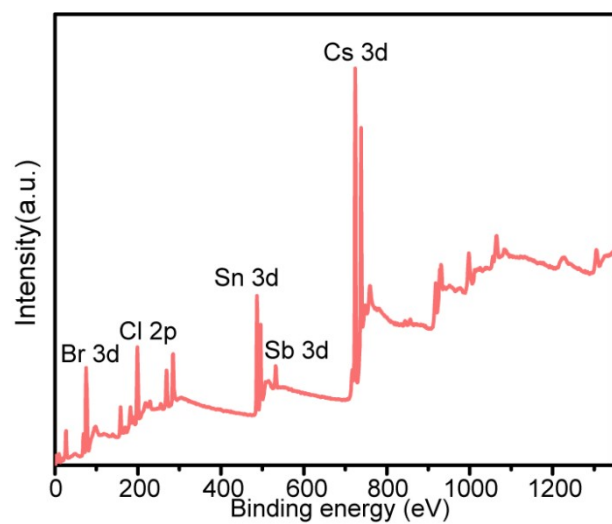


Fig. S2. XPS survey spectrum of sample $\text{Cs}_2\text{SnCl}_4\text{Br}_2$: Sb.

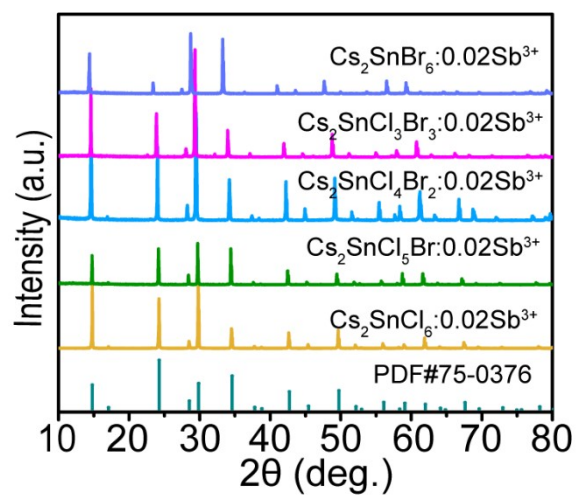


Fig. S3. XRD patterns $\text{Cs}_2\text{SnCl}_x\text{Br}_y: 0.02\text{Sb}$ ($x+y=6$) and the standard XRD pattern of Cs_2SnCl_6 (PDF#75-0376).

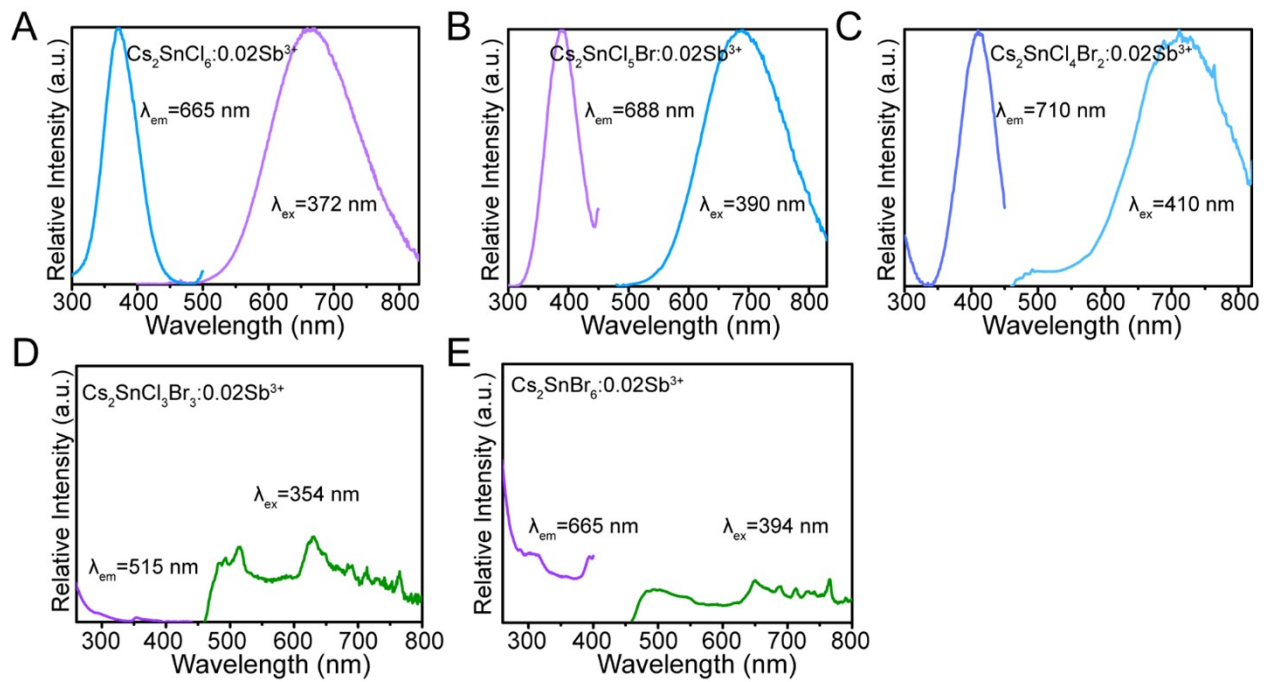


Fig. S4. Excitation and emission spectra of the as-synthesized $\text{Cs}_2\text{SnCl}_x\text{Br}_y:0.02\text{Sb}$ ($x+y=6$) phosphors.

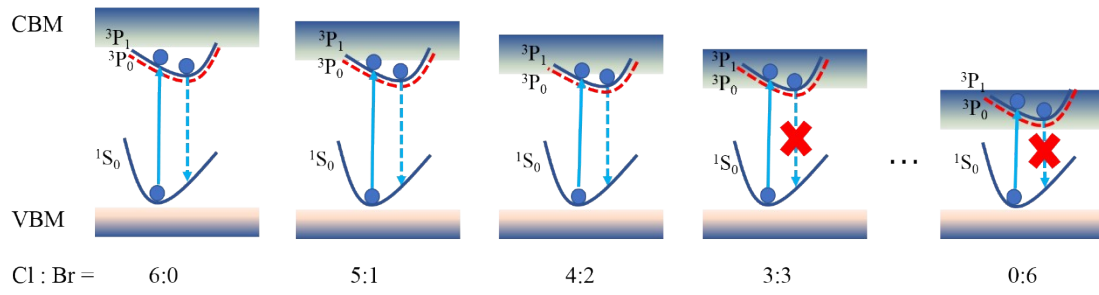


Fig. S5. The bandgap and energy level diagram of Sb^{3+} -doped $\text{Cs}_2\text{SnCl}_x\text{Br}_y$ ($x+y=6$).

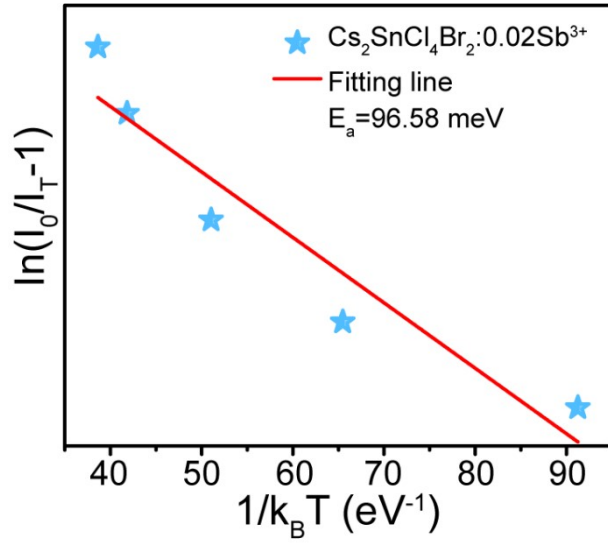


Fig. S6. The relationships between $\ln(I_0/I_T - 1)$ versus $1/k_B T$ ($T=77\text{--}300 \text{ K}$) and the linear fitting result.

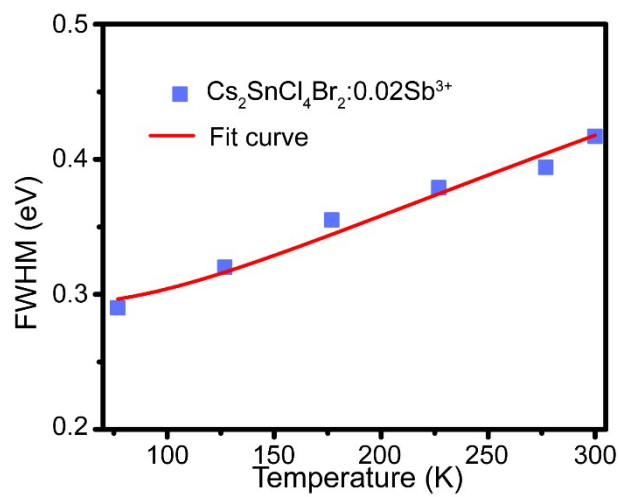


Fig. S7. Temperature dependence of PL FWHM of $\text{Cs}_2\text{SnCl}_4\text{Br}_2: 0.02\text{Sb}^{3+}$.

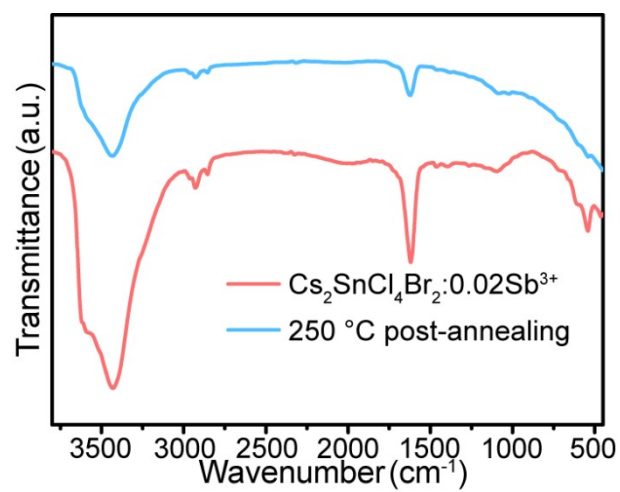


Fig. S8. FT-IR of the sample Cs₂SnCl₄Br₂: 0.02Sb before and after post-annealing at 250 °C.

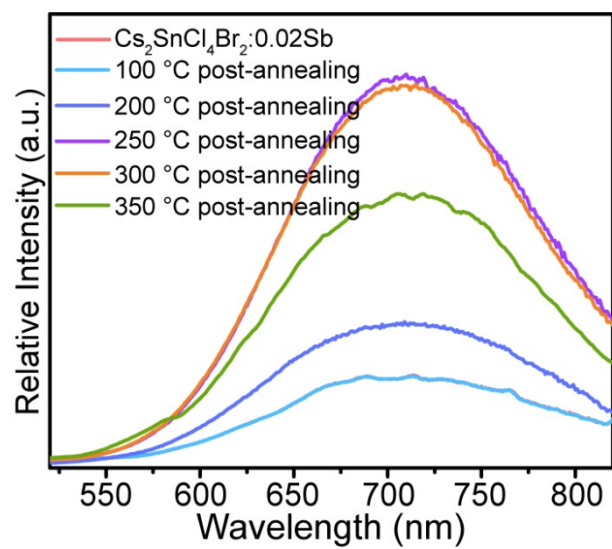


Fig. S9. Emission spectra of $\text{Cs}_2\text{SnCl}_4\text{Br}_2:0.02\text{Sb}$ on post-annealing temperature.

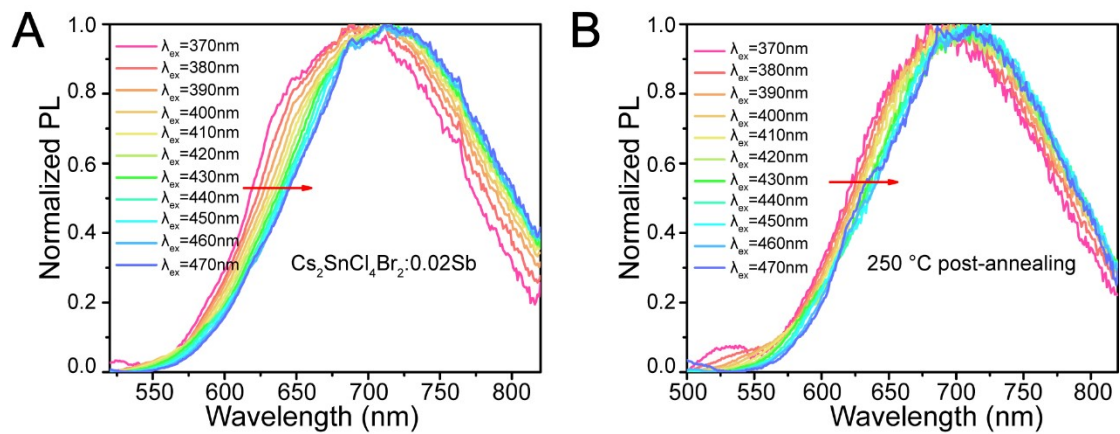


Fig. S10. Emission spectra of the original (A) and post-annealed (at 250 °C) (B) sample $\text{Cs}_2\text{SnCl}_4\text{Br}_2:0.02\text{Sb}$ under different excitations varied from 370 to 470 nm.

Table S1. The calculated crystallographic data and refinement parameters.

Atoms	Sites	x	y	z	Frac.
Cs1	8c	0.2500	0.2500	0.2500	1.0000
Sn1	4a	0.0000	0.0000	0.0000	1.0000
Cl1	24e	0.2388	0.0000	0.0000	0.7174
Br1	24e	0.2388	0.0000	0.0000	0.3840

Crystal system: centric F-centered cubic

Space group: Fm-3m

Z=4

Lattice parameters: a=b=c=10.4663

Reliable factors: $R_{wp}=9.42\%$, $R_p=6.67\%$, $\chi^2=3.213$

Table S2. The chemical composition data of Cs₂SnCl₄Br₂: 0.02Sb measured by EDS.

Cs (%)	Sn (%)	Cl (%)	Br (%)	Sb (%)	Total atomic (%)
25.85	11.21	49.94	12.66	0.33	100
Theoretical atomic ratio: Cs: Sn: Cl: Br: Sb =2: 1: 4: 2: 0.02					
Experimental ratio: Cs: Sn: Cl: Br: Sb =2.31: 1: 4.45: 1.13: 0.03					

Table S3. The summary of PLQY and FWHM of the reported NIR halide perovskites.

	Samples	Emission peaks	FWHM	PLQY	Years
		[nm]	[nm]	(%)	
Pb- based	$\text{CH}_3\text{NH}_3\text{PbI}_3$	765	50	17	2014 ¹
	$\text{CH}_3\text{NH}_3\text{PbI}_{3-a}\text{Cl}_a$	765	50	30	
	FAPbI ₃	770-780	45	>70	2017 ²
	CsPbI ₃	695	50	65	2017 ³
	$\text{CsSn}_x\text{Pb}_{1-x}\text{I}_3$	700-850	100	0.3-3	2017 ⁴
	$\text{Cs}_x\text{FA}_{1-x}\text{PbI}_3$	650-800	50	60-70	2018 ⁵
	$\text{PEA}_2\text{Pb}_{1-x}\text{Sn}_x\text{I}_4$	710	154	6	2019 ⁶
	$\text{CsSn}_x\text{Pb}_{1-x}\text{I}_3$: Na	830	100	28	2020 ⁷
	MAPbI ₃	774	50	---	2020 ⁸
Pb-free	CsSnI ₃	950	80	0.06	2016 ⁹
	MASnI ₃	870	85	---	2017 ¹⁰
	{en}MASnI ₃	890	100	---	
	FASnI ₃	880	120	---	2019 ¹¹
	Cs ₂ AgInCl ₆ :	996	50	0.2	2019 ¹²
	Yb/Er	1537	60	0.02	
	Cs ₃ Sb ₂ I ₉	750	120	---	2019 ¹³
	Cs ₂ AgInCl ₆ : Bi/Er	1540	50	---	2020 ¹⁴
	Cs ₂ AgInCl ₆ : Bi/Yb	994	60	---	
Cs ₂ SnCl ₄ Br ₂ : Sb	710	164	8.11	This work	

Table S4 Photoelectric parameters of the NIR-LEDs fabricated using the samples Cs₂SnCl₄Br₂: 0.02Sb with (NIR-LED-1) and without post-annealing (NIR-LED-2).

NIR-LEDs	Current (mA)	Voltage (V)	NIR power (mW)	Photoelectric efficiency (%)
NIR-LED-1	19.98	2.95	1.925	3.264
	29.96	2.971	2.887	3.243
	39.97	2.987	3.815	3.195
	49.97	3.003	4.696	3.131
	59.97	3.015	5.564	3.078
	69.98	3.027	6.353	2.999
	79.98	3.039	7.16	2.947
	89.98	3.05	7.882	2.872
	99.99	3.061	8.603	2.811
	149.9	3.112	11.76	2.520
	199.9	3.159	14.28	2.261
	250	3.206	16.13	2.012
	299.8	3.25	17.23	1.768
	NIR-LED-2	20	2.945	1.498
29.98		2.964	2.261	2.544
39.98		2.981	3.005	2.521
49.96		2.995	3.713	2.482
59.97		3.008	4.396	2.437
69.97		3.02	5.06	2.395
79.97		3.032	5.725	2.361
89.98		3.042	6.328	2.311
99.99		3.053	6.97	2.283
149.9		3.102	9.706	2.086
199.9		3.149	12.05	1.914
250		3.194	13.85	1.734
299.9		3.239	15.33	1.578

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