

Electronic supplementary information

Double perovskite Cs₂NaInCl₆ nanocrystals with intense dual-emission via self-trapped exciton to Tb³⁺ dopant energy transfer

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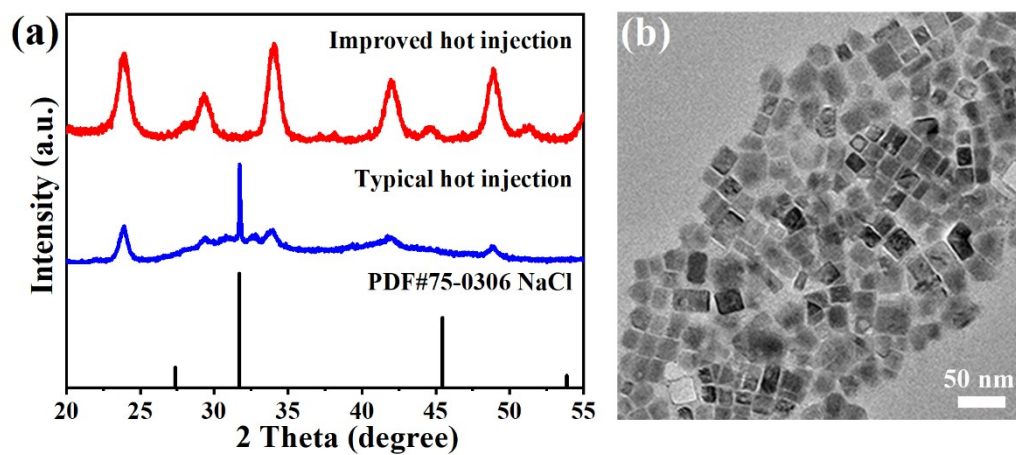


Fig. S1 (a) XRD patterns of Cs₂NaInCl₆ NCs prepared by typical hot injection compared with these synthesized by improved hot injection. (b) TEM image of Cs₂NaInCl₆ NCs prepared by typical hot injection, showing irregular morphology.

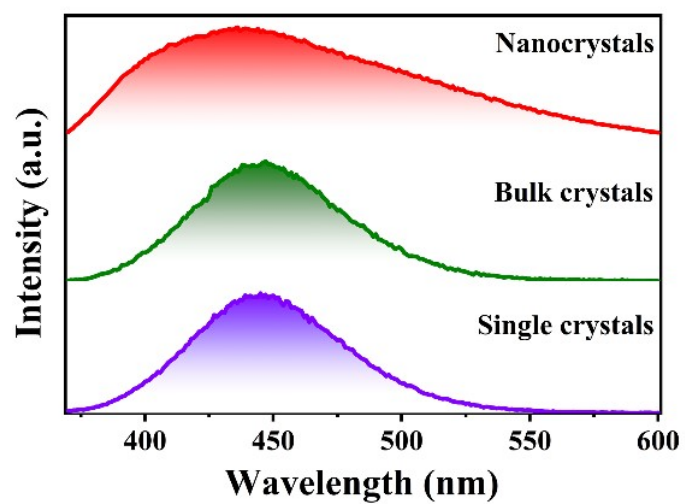


Fig. S2 PL spectra of Cs₂NaInCl₆ nanocrystals, bulk crystals, and single crystals (excited at 320 nm).

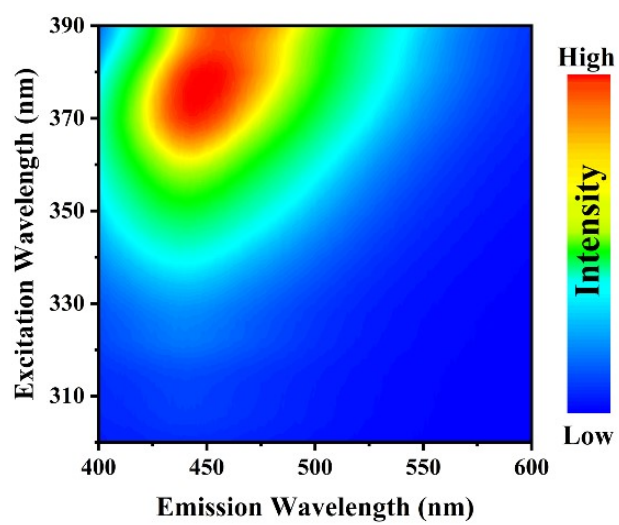


Fig. S3 Excitation-emission color map of surface ligand.

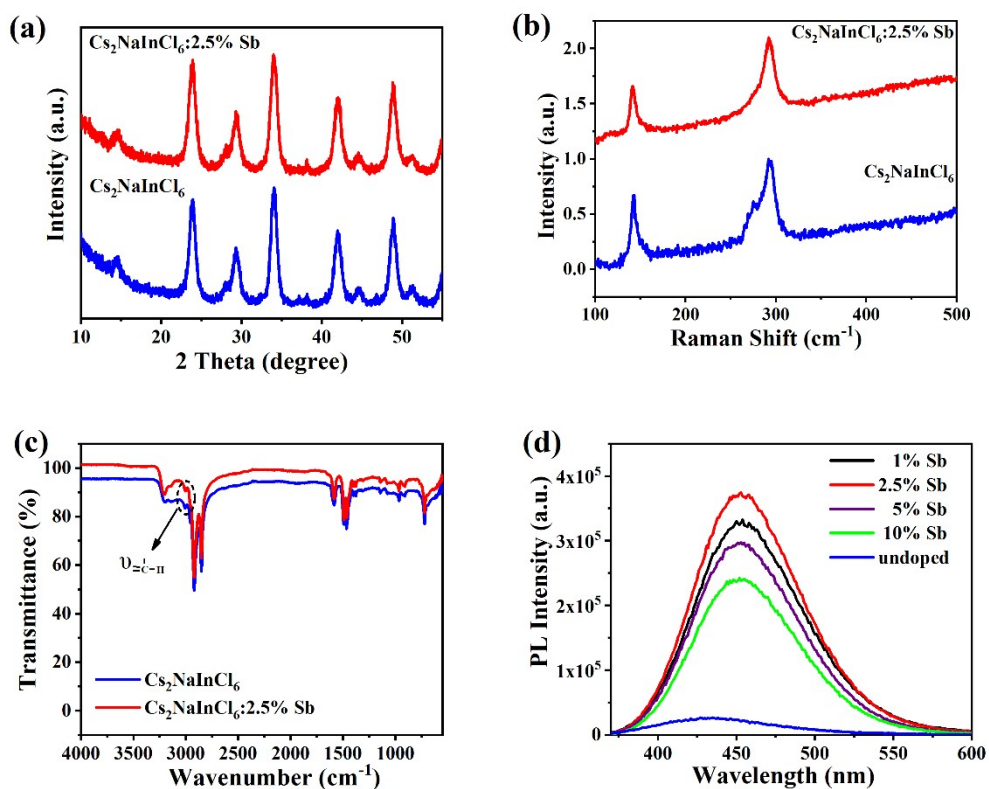


Fig. S4 (a) XRD patterns of $\text{Cs}_2\text{NaInCl}_6$ and $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb}$ NCs. (b) Raman spectra of $\text{Cs}_2\text{NaInCl}_6$ and $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb}$ NCs collected at 532 nm green laser source. The peaks at 292 and 142 cm^{-1} can be corresponded to the stretching (A_{1g}) and bending (T_{2g}) modes of $[\text{InCl}_6]^{3-}$ octahedron, respectively. (c) FT-IR spectra of $\text{Cs}_2\text{NaInCl}_6$ and $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb}$ NCs. It could be observed that the characteristic peak of the cis-unsaturated $=\text{C}-\text{H}$ stretching vibration in OA and OAm at 3006 cm^{-1} for both $\text{Cs}_2\text{NaInCl}_6$ and $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb}$ NCs. (d) PL spectra (excited by 335 nm) of undoped and Sb-doped $\text{Cs}_2\text{NaInCl}_6$ NCs, as framed in the figures.

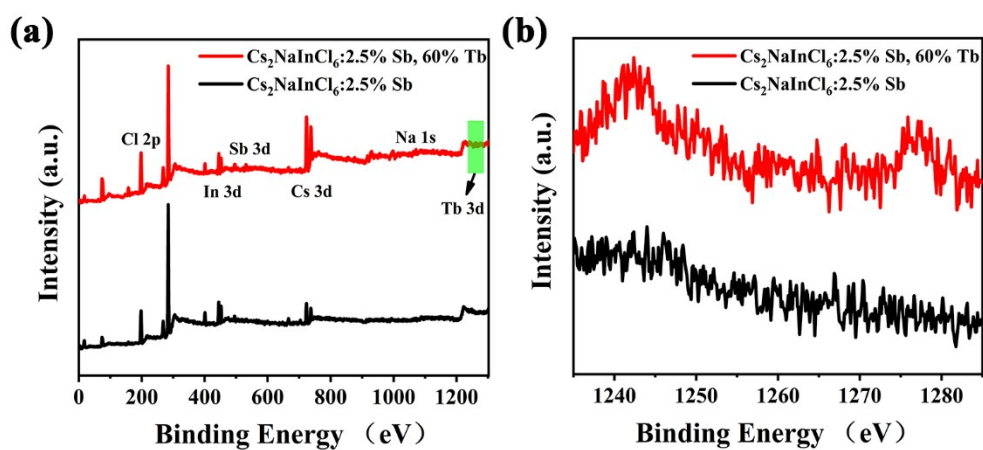


Fig. S5 (a) Survey XPS spectra of $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb}$ and $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb},60\%\text{Tb}$ NCs. (b) High-resolution XPS spectrum of Tb 3d in $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb},60\%\text{Tb}$.

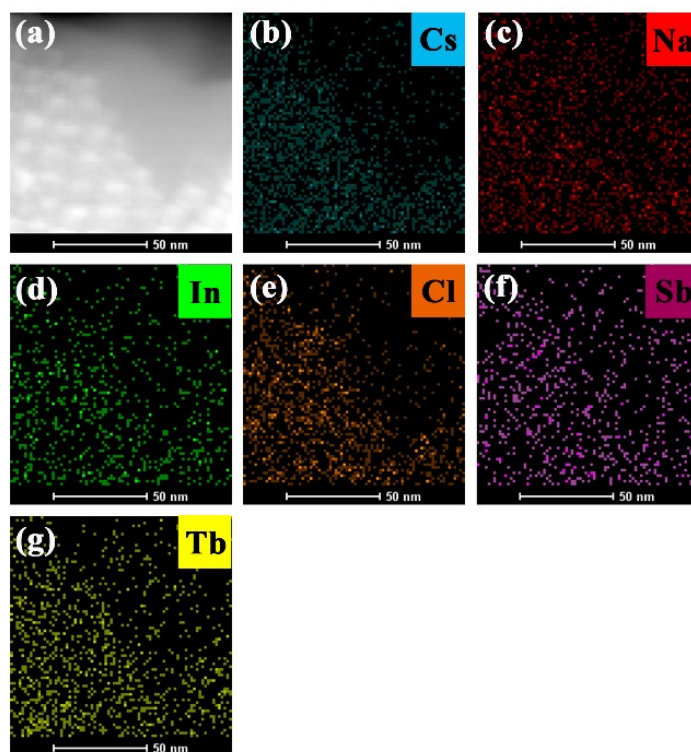


Fig. S6 (a) High-angle annular dark-field (HAADF) image of $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb},60\%\text{Tb}$ NCs. (b-g) STEM-EDS elemental mappings of Cs^+ , Na^+ , In^{3+} , Cl^- , Sb^{3+} , Tb^{3+} colocalized in $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb},60\%\text{Tb}$ NCs.

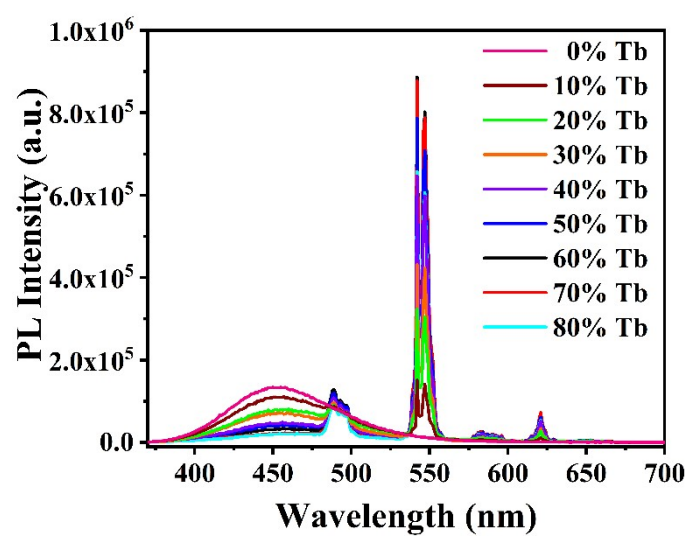


Fig. S7 PL spectra of Cs₂NaInCl₆:2.5%Sb,(0%-80%)Tb NCs excited at 335 nm, as framed in the figure.

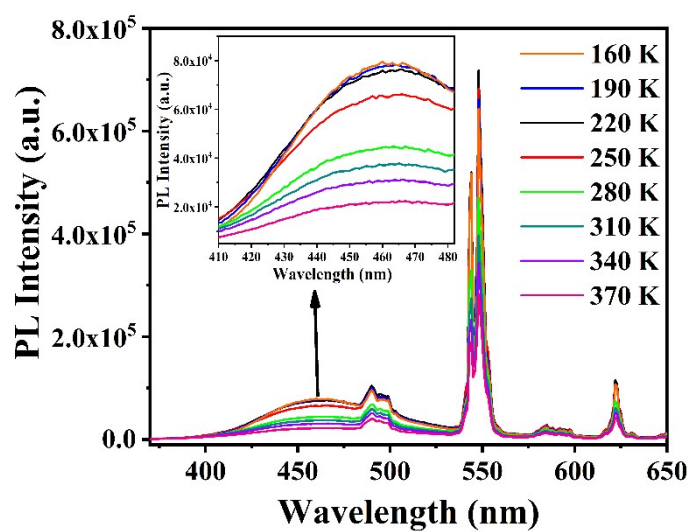


Fig. S8 PL spectra of $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb},30\%\text{Tb}$ NCs at different temperature. With the increase of temperature, the STEs emission gradually decrease. While the intensity of Tb^{3+} ions emission is enhanced as the temperature increases from 160 K to 220 K, and then weakens when the temperature increases from 220 K to 370 K.

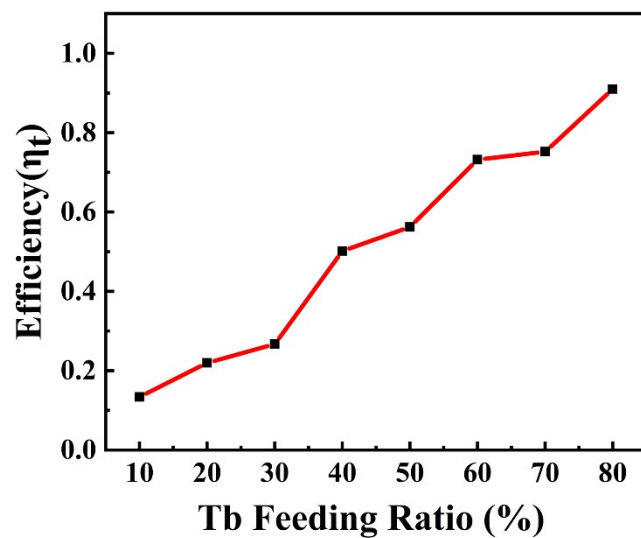


Fig. S9 The energy transfer efficiency variation of $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb},(10\%-80\%)\text{Tb}$ (monitored at 450 nm) under excitation at 335 nm as a function of Tb feeding ratio.

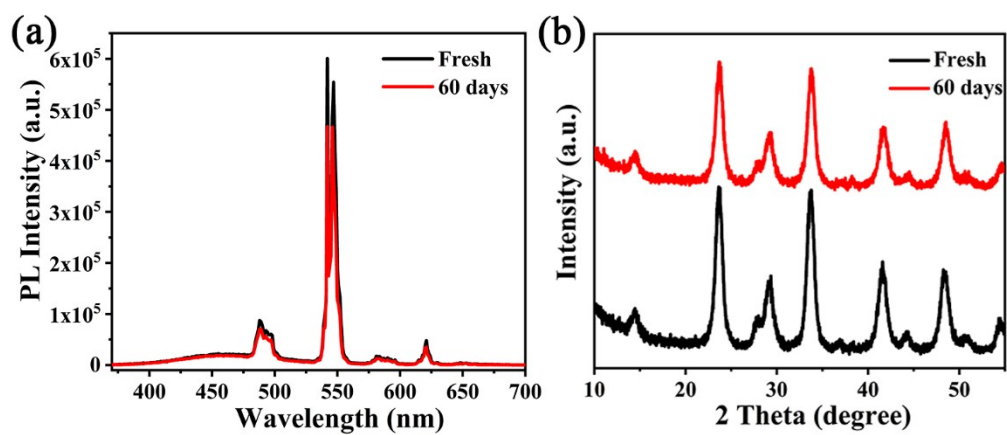


Fig. S10 (a) PL spectra and (b) XRD patterns of fresh $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb},60\%\text{Tb}$ NCs (black) and $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb},60\%\text{Tb}$ NCs stored in air for 60 days (red).

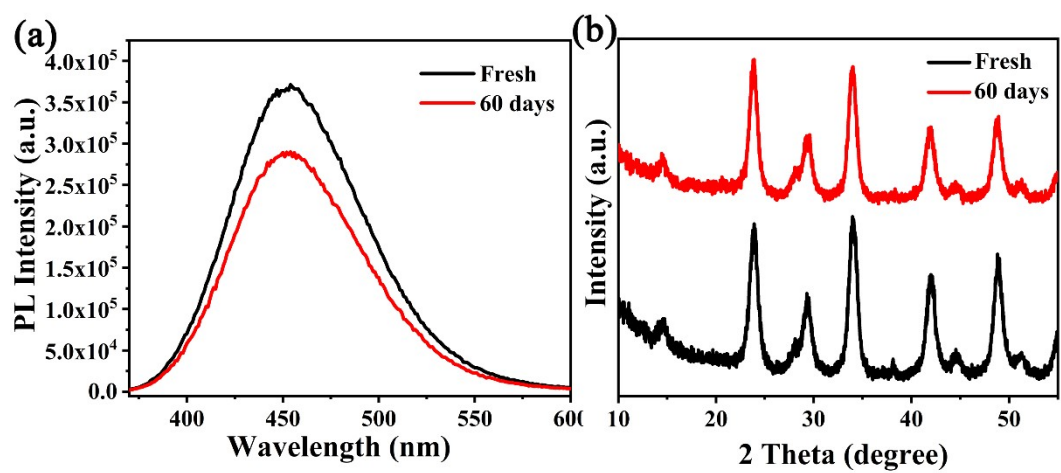


Fig. S11 (a) PL spectra and (b) XRD patterns of fresh $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb}$ NCs (black) and $\text{Cs}_2\text{NaInCl}_6:2.5\%\text{Sb}$ NCs stored in air for 60 days (red).

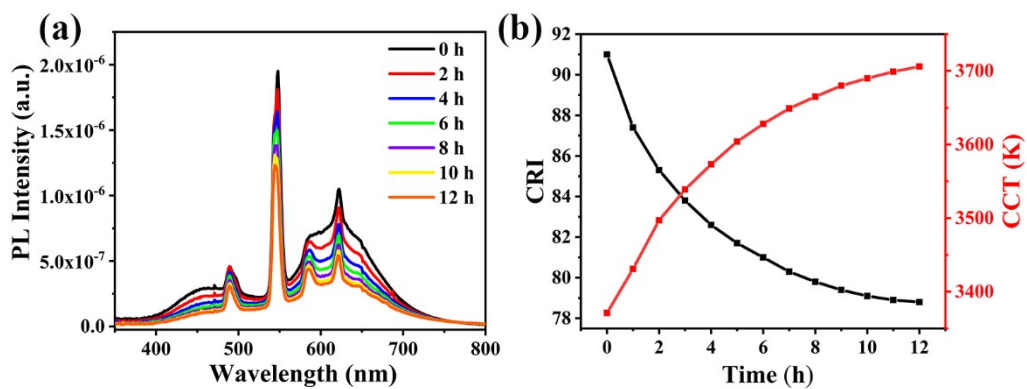


Fig. S12 (a) Evolution of PL spectra of WLED device after different running periods at the same bias and measurement conditions (at 20 mA). (b) CRI and CCT of the WLED measured at different working time.

Table S1. Inductively coupled plasma optical emission spectrometer (ICP-OES) data of Cs₂NaInCl₆:Sb,Tb NCs.

Feeding ratios x of Tb/(Tb+Sb+In)×100%	Tb/(Tb+Sb+In) ratios measured by ICP	Sb/(Sb+In) ratios measured by ICP
0%	0%	1.1%
10%	1.9%	1.3%
20%	9.0%	1.3%
30%	13.1%	1.4%
40%	25.7%	1.3%
50%	31.5%	1.4%
60%	43.6%	1.4%
70%	49.0%	1.5%
80%	52.4%	1.5%

Table S2. Comparison of PLQY of reported lead-free perovskite NCs with that of this work.

Lead-free perovskite NCs	PLQY (%)	Reference
Cs ₂ NaInCl ₆ :2.5%Sb, 60%Tb	74%	This work
Cs ₂ NaInCl ₆ :10%Ag	31.1%	30
Cs ₂ AgInCl ₆ :1%Bi	11.4%	29
Cs ₂ NaBiCl ₆	~16%	10
Bi-doped Cs ₂ Ag _{0.4} Na _{0.6} InCl ₆	~22%	14
Cs ₂ NaBiCl ₆ :14%Mn	3.9%	34

Table S3. Inductively coupled plasma optical emission spectrometer (ICP-OES) data of Cs₂NaInCl₆:2.5%Sb,45%Tb,3%Mn NCs.

Tb/(Tb+Sb+In+Mn) ratios	Mn/(Tb+Sb +In+Mn) ratios	Sb/(Sb+In) ratios
34.3%	1.4%	1.6%