

Supporting Information

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Experimental

1. Chemicals

1-octadecene (ODE, 90%), oleic acid (OA, 90%), oleylamine (OAm, 70%), cyclohexane, lead chloride (PbCl_2), manganese chloride (MnCl_2), antimony trichloride (SbCl_3), and toluene, ethyl acetate. All chemicals were directly used without further purification.

2. Preparation of Cs-oleate

0.407g of Cs_2CO_3 , 10 ml of ODE, and 1.25 ml OA were loaded into a 20 ml glass bottle. The mixture was heated for 1h at 130 °C until Cs_2CO_3 was completely dissolved to form a clear solution.

3. Synthesis of the Mn^{2+} doped or Mn^{2+} and Sb^{3+} co-doped CsPbCl_3 NCs. The Mn^{2+} doped or Mn^{2+} and Sb^{3+} co-doped CsPbCl_3 NCs were synthesized by hot injection method. In a typical synthesis, 0.375 mmol of PbCl_2 , MnCl_2 (and SbCl_3), ODE (10 ml), OA (1ml), and OAm (1ml) were loaded into a 100 ml three-necked flask and heated at 130°C for 1h under N_2 atmosphere. Then the reaction temperature of the mixture was increased to 180°C and 1 ml of the Cs-oleate precursor was rapidly injected. After that, the mixture solution was kept at 180°C for 30s. Then, the reaction solution was cooled in cold water. The Mn^{2+} , Sb^{3+} co-doped CsPbCl_3 NCs were obtained by regulating the molar feed ratio of $\text{MnCl}_2/\text{SbCl}_3$.

Characterization: TEM images were collected by Hitachi H-800 at 200KV. HRTEM and mapping were measured by JEM-2100F at 200KV. Absorption spectra were collected with UV/vis- spectrophotometer (Shimadzu UV-1800). Photoluminescence spectra were recorded on a Shimadzu RF-6000 spectrofluorometer. X-Ray Diffraction (XRD) patterns were measured by using a Bruker D8 diffractometer with $\text{Cu K}\alpha$ radiation. Time-resolved emission decay curves were measured using a PLS980 time correlated single-photon counting (TCSPC) system. Low-temperature fluorescence spectroscopy was acquired using a tuneable optical parameter oscillator (OPO) as the excitation source and a visible photomultiplier (350–850 nm) combined with a double-grating monochromator for spectral collection. X-ray photoelectron spectroscopy (XPS) was collected by Kratos Axis UltraDLD. Absolute emission QY values were measured at room temperature using a commercial integrating sphere installed in FLS980 spectrometer from Edinburgh Instruments. Calibration of the photoluminescence QY value was performed using the standard sample $\text{YAG}:\text{Ce}^{3+}$ (BM302D, Jiangsu Bree Optonics Co., Ltd, peaking at 551 nm).

Calculation method

First-principle calculations were performed by the density functional theory (DFT) using the Vienna Ab-initio Simulation Package (VASP) package.¹ The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional were used to describe the electronic exchange and correlation effects.² Uniform G-

centered k-points meshes with a resolution of $2\pi \cdot 0.04 \text{ \AA}^{-1}$ and Methfessel-Paxton electronic smearing were adopted for the integration in the Brillouin zone for geometric optimization. The simulation was run with a cutoff energy of 500 eV throughout the computations. These settings ensure convergence of the total energies to within 1 meV per atom. Structure relaxation proceeded until all forces on atoms were less than 1 meV \AA^{-1} and the total stress tensor was within 0.01 GPa of the target value. For the Mn^{2+} - and Sb^{3+} -doped CsPbCl_3 structure, CsPbCl_3 with tetragonal structure (space group: $P4mm$) was selected, and then we build a $2 \times 2 \times 2$ supercell structure based on CsPbCl_3 unit cell, in which one Pb atom was replaced by Mn and the other Pb atom was replaced by Sb.

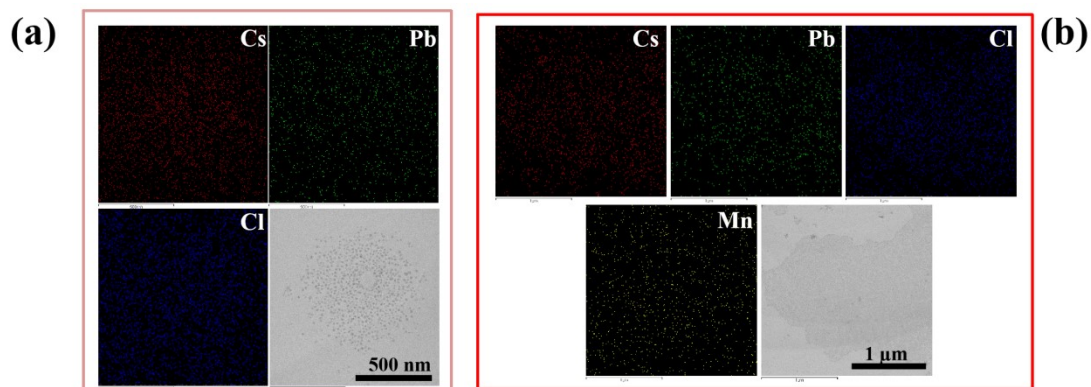


Fig. S1. EDS mapping images for (a) CsPbCl_3 , (b) $\text{CsPbCl}_3:\text{Mn}^{2+}$. It can be seen that the elements in each material are evenly distributed.

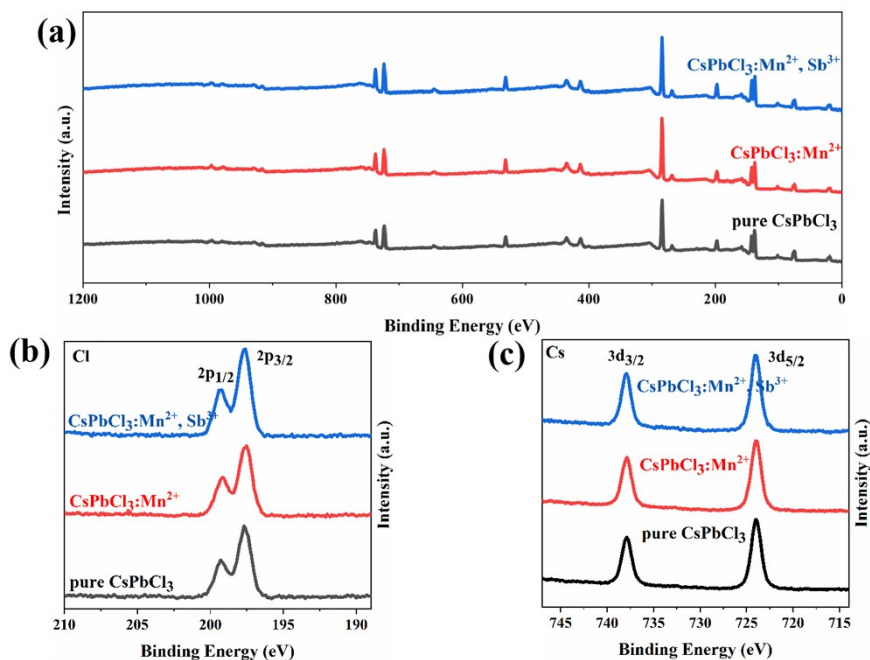


Fig. S2. (a) XPS total patterns, high-resolution XPS analysis of (b) Cl 2p and (c) Cs 3d for pure CsPbCl_3 , $\text{CsPbCl}_3:\text{Mn}^{2+}$ and $\text{CsPbCl}_3:\text{Mn}^{2+}, \text{Sb}^{3+}$ respectively.

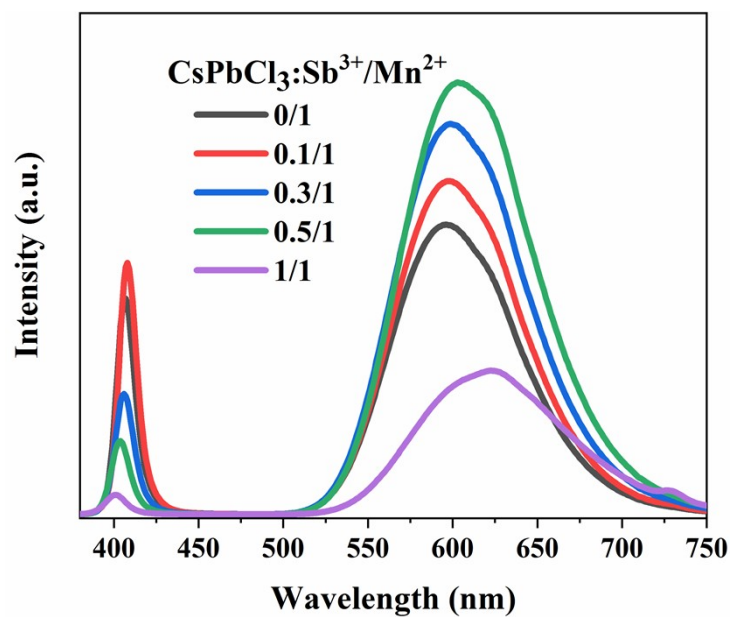


Fig. S3. Steady-state PL spectra for CsPbCl₃ NCs with varied the molar ratio of Sb³⁺/Mn²⁺ upon the excitation of 365 nm source.

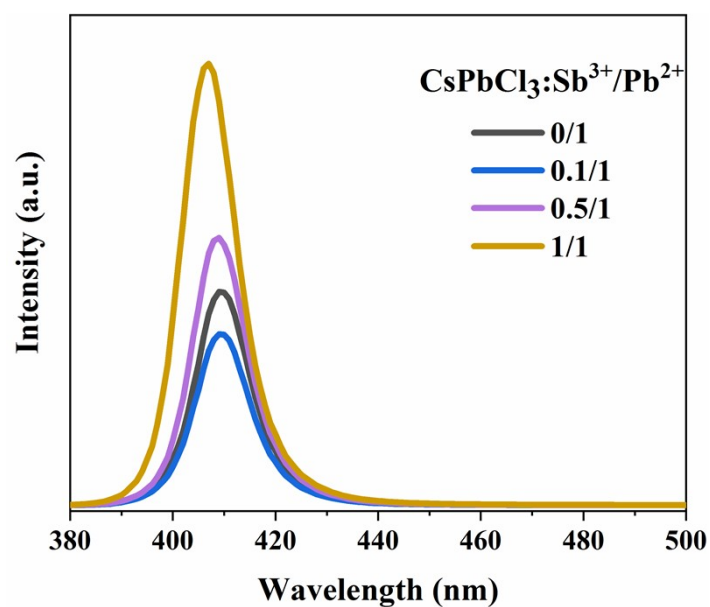


Fig. S4. PL spectra of CsPbCl₃ NCs with only Sb³⁺ doping and changing the Sb³⁺/Pb²⁺ molar ratio under excitation at 365 nm .

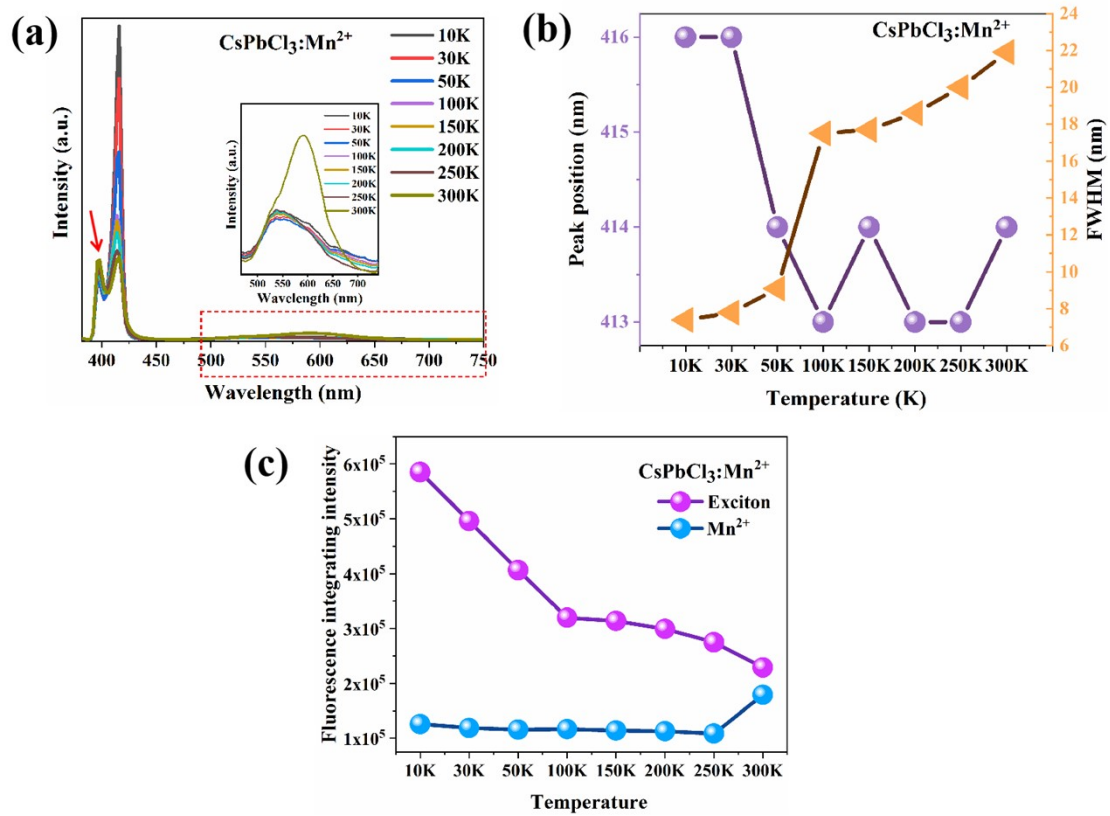


Fig. S5. (a) Temperature-dependent steady-state spectra (inset: enlarged image inside the dashed box) and (b) corresponding peak position and FWHM curves for CsPbCl₃:Mn²⁺ sample. (c) The plot of integrated PL intensity as a function of temperature for CsPbCl₃:Mn²⁺ sample.

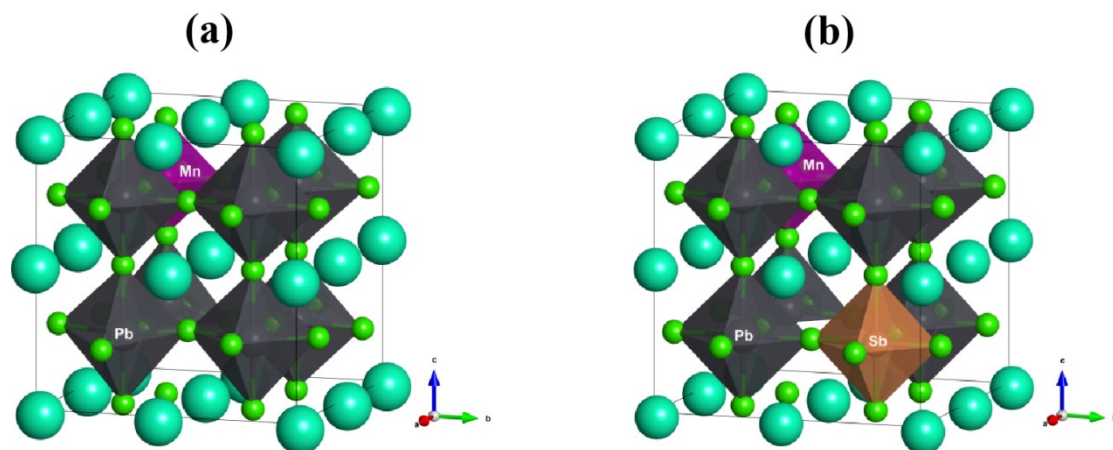


Fig. S6. The optimized structure of (a) CsPbCl₃:Mn²⁺ and (b) CsPbCl₃:Mn²⁺, Sb³⁺ structures.

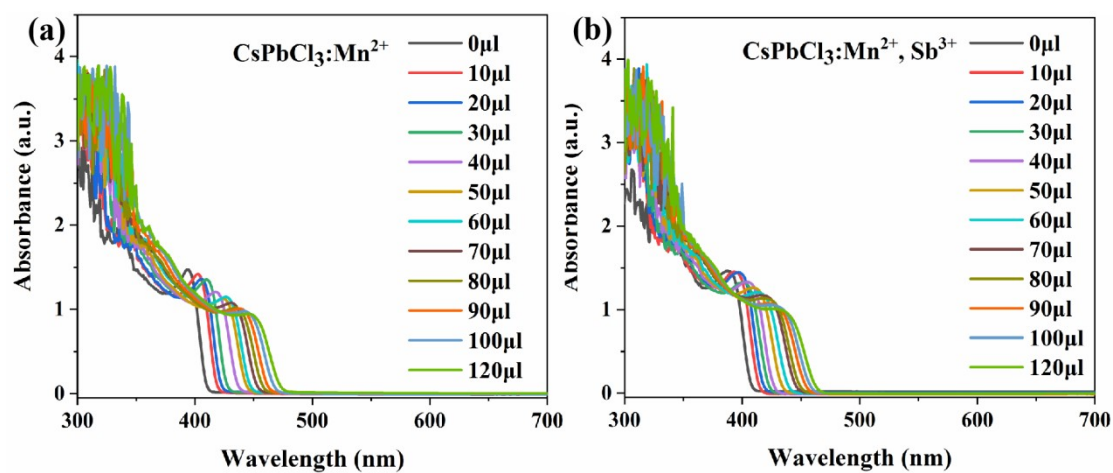


Fig. S7. Absorption spectra of (a) $\text{CsPbCl}_3:\text{Mn}^{2+}$ and (b) $\text{CsPbCl}_3:\text{Mn}^{2+}, \text{Sb}^{3+}$ samples after anion exchange with varying amounts of PbBr_2 .

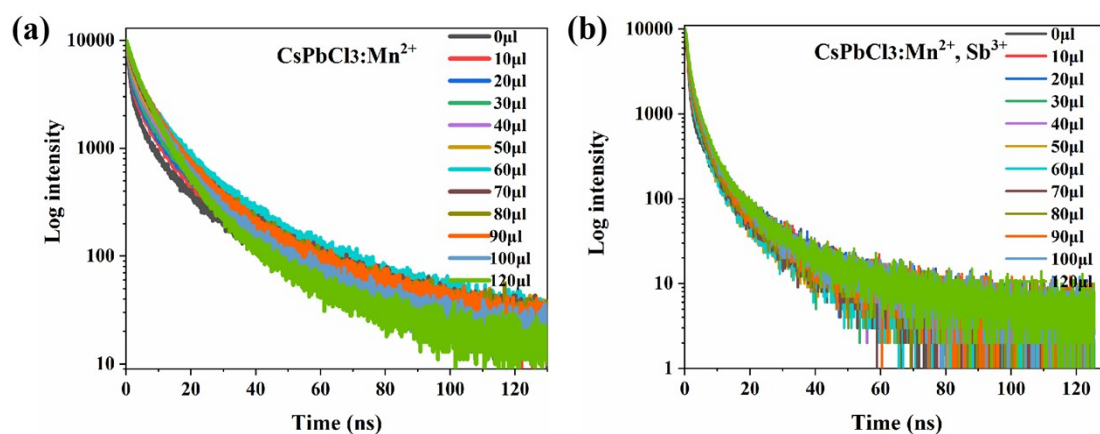


Fig. S8. Time-resolved PL spectra of exciton emission for (a) $\text{CsPbCl}_3:\text{Mn}^{2+}$ and (b) $\text{CsPbCl}_3:\text{Mn}^{2+}, \text{Sb}^{3+}$ samples.

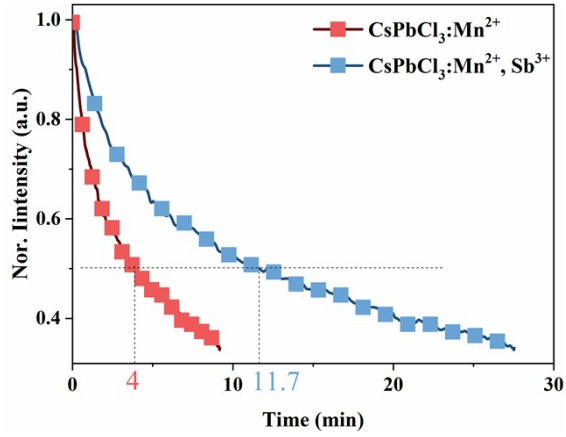


Fig. S9. Device stability for CsPbCl₃:Mn²⁺ (red) and CsPbCl₃:Mn²⁺, Sb³⁺ (blue) samples.

Table S1. Average lifetime data of Mn²⁺ after single exponential fit for CsPbCl₃ NCs with different feed molar ratio of Mn²⁺/Sb³⁺.

Mn/Sb	0.3/0	0.5/0	0.1/0.5	0.3/0.5	0.5/0.5
T_{ave}/ms	1.63	1.73	1.70	1.68	1.67

Table S2. Emission decay of exciton for CsPbCl₃ NCs with different molar ratios of Mn²⁺/Sb³⁺.

Mn²⁺/Sb³⁺	0.1/0	0.3/0	0.5/0	0.1/0.5	0.3/0.5	0.5/0.5
A1	9028.43	8526.48	8722.90	9064.97	9773.19	11054.68
T₁/ns	1.38	1.31	1.21	1.07	0.95	0.99
A2	1511.07	2067.68	1987.23	1648.21	1001.16	533.07
T₂/ns	16.0	10.39	8.04	8.15	5.37	4.41
T_{ave}/ns	10.96	10.39	8.04	8.15	5.37	4.41

Table S3. Summary of the performance of Violet LEDs.

Emission layer materials	EL peak position (nm)	Max EQE (%)	Luminance (cd/m²)	Ref
Cs ₃ Sb ₂ Br ₉ QDs	408	0.21	29.60	37
Cs ₃ CeBr ₆ crystal	391	0.46	-	38
CsPbCl ₃ :Mg NCs	402	0.1	135	39
CsPbCl ₃ :Mn ²⁺ , Sb ³⁺ NCs	413	0.39	121	This work

References:

1. Kresse. G.; Furthmuller. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *J. Comput. Mater. Sci.*, 1996, **6**, 15–50.
2. Perdew. J. P.; Burke. K.; Ernzerhof. M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.*, 1996, **77**, 3865–3868.