

## Supporting Information

### Tunable photoluminescence in $\text{Sb}^{3+}$ -doped zero-dimensional hybrid metal halides with intrinsic and extrinsic self-trapped excitons

Jun Zhou<sup>†</sup>, Mingze Li<sup>‡</sup>, Maxim S. Molokeev<sup>§, †, Δ</sup>, Jiayue Sun<sup>†</sup>, Denghui Xu<sup>\*, †</sup>, and Zhiguo Xia<sup>\*, ‡, ◇</sup>

<sup>†</sup> School of Science, Beijing Technology and Business University, Beijing 100048, P. R. China

<sup>‡</sup> The Beijing Municipal Key Laboratory of New Energy Materials and Technologies, School of Materials Sciences and Engineering, University of Science and Technology Beijing, Beijing, 100083, China

<sup>§</sup> Laboratory of Crystal Physics, Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Krasnoyarsk 660036, Russia

<sup>Δ</sup> Siberian Federal University, Krasnoyarsk, 660041, Russia

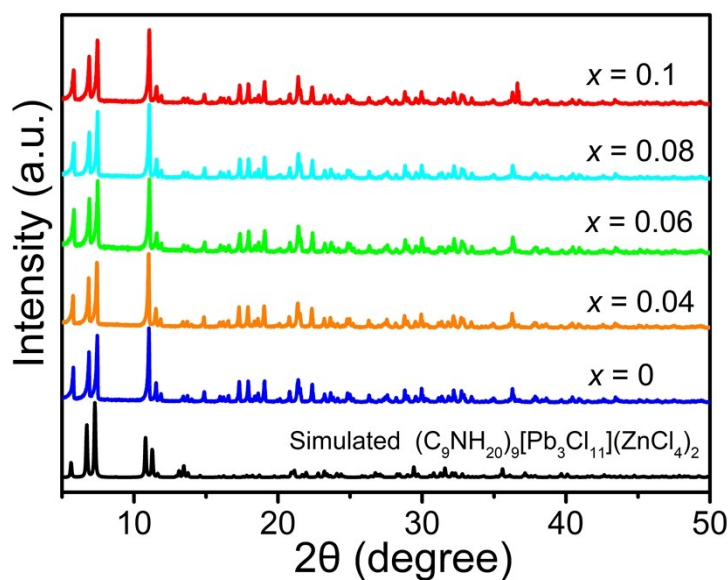
<sup>Δ</sup> Department of Physics, Far Eastern State Transport University, Khabarovsk, 680021, Russia

<sup>◇</sup> State Key Laboratory of Luminescent Materials and Devices and Institute of Optical Communication Materials, South China University of Technology, Guangzhou, 510641, China

Corresponding Author

\*[xiazg@scut.edu.cn](mailto:xiazg@scut.edu.cn)

\*[xudh@btbu.edu.cn](mailto:xudh@btbu.edu.cn)



**Fig. S1.** The simulated and experimental X-ray powder patterns of  $(\text{C}_9\text{NH}_{20})_9[\text{Pb}_3\text{Cl}_{11}](\text{ZnCl}_4)_2 \cdot \text{Sb}^{3+}$  with different  $\text{Sb}^{3+}$  contents.

**Table S1.** The crystal structure parameters of  $(\text{C}_9\text{NH}_{20})_9[\text{Pb}_3\text{Cl}_{11}](\text{ZnCl}_4)_2$ .

Formula moiety	$(\text{C}_9\text{NH}_{20})_9[\text{Pb}_3\text{Cl}_{11}](\text{ZnCl}_4)_2$
Molecular weight	2670.74
Temperature (K)	296
Space group, $Z$	$P31c$ , 2
$a$ (Å)	14.8386 (0)
$c$ (Å)	30.6974 (13)
$V$ (Å <sup>3</sup> )	5853.5331 (6)
$\rho_{\text{calc}}$ (g/cm <sup>3</sup> )	1.441
$2_{\text{max}}$ (°)	46.4
$R1 [F_o > 4\sigma(F_o)]$	0.0735
$wR2$	0.231
$Goof$	1.116

## References

- (1) Sheldrick, G. M., A short history of SHELX. *Acta Crystallogr A* **2008**, *64* (Pt 1), 112-22.
- (2) Brandenburg, K.; Berndt, M. J. G. S., DIAMOND: Visual Crystal Structure Information System CRUSTAL IMPACT, Postfach 1251, D-53002 Boon. **2004**.
- (3) TOPAS, V. J. T. i. n. c. r. f. t. r., 2: General profile and structure analysis software for powder diffraction data–User's Manual; Bruker AXS: Karlsruhe, Germany. **2008**. **2002**.