

## Supporting Information

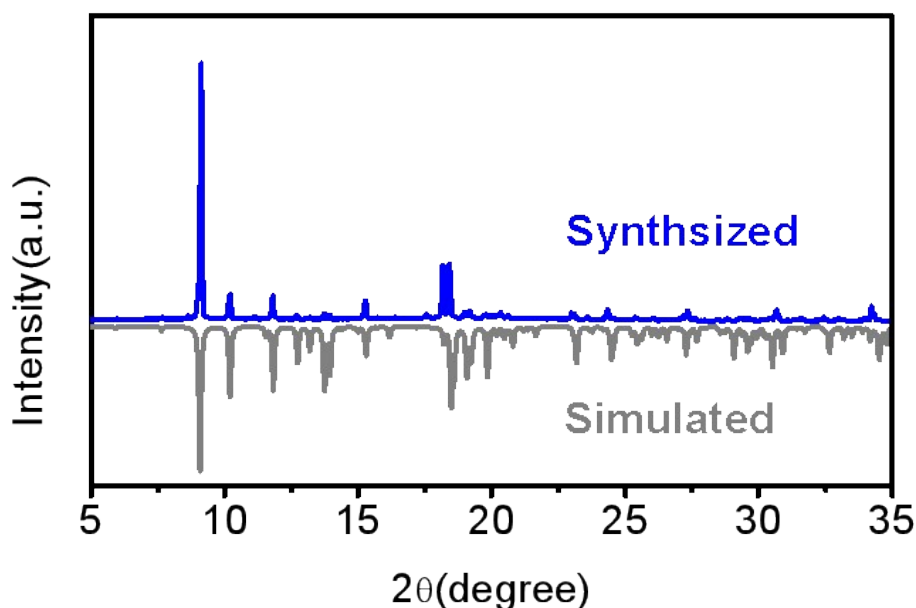
# Antimony Doping Indium-based Halide Single Crystals Enabling White-light Emission

Yue Wu,<sup>a</sup>Cui-Mi Shi,<sup>b</sup> Shi-Rong Kang<sup>a</sup> and Liang-Jin Xu,<sup>b,c\*</sup>

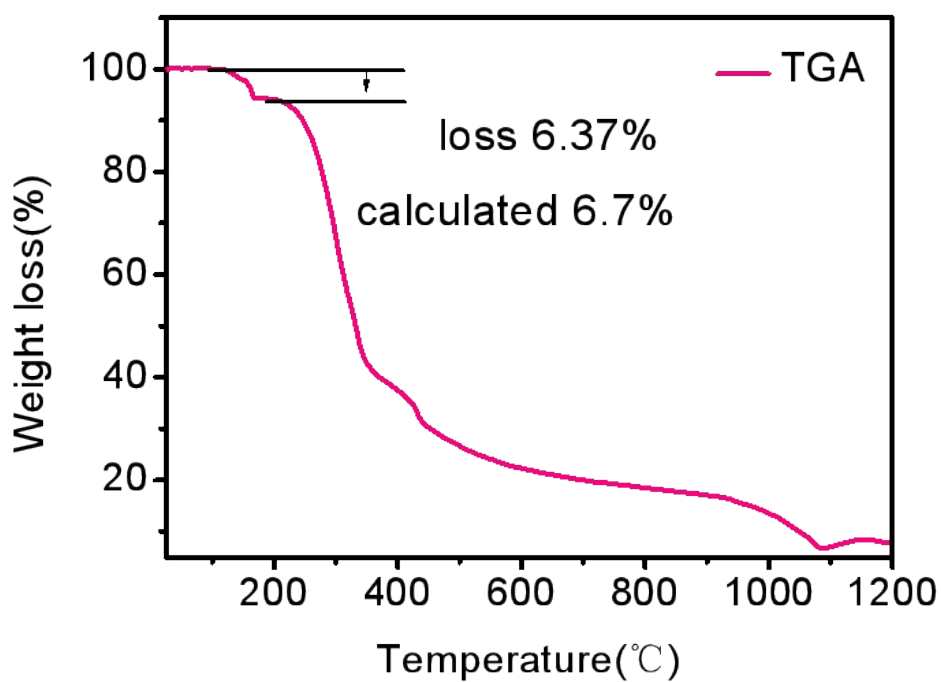
<sup>a</sup>School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng, Shandong,252000, China

<sup>b</sup>State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China

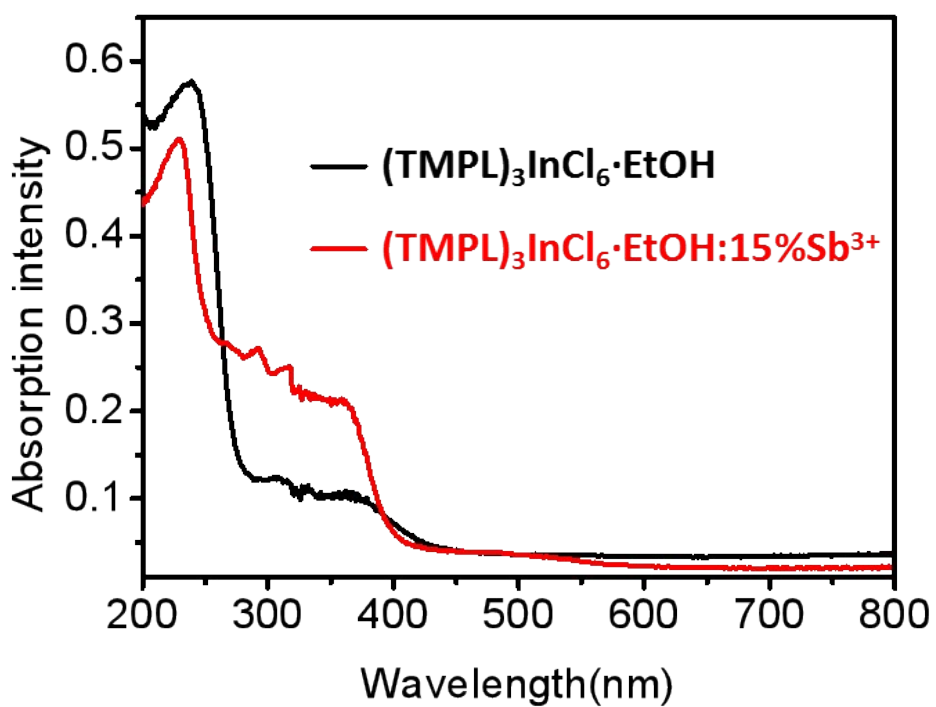
<sup>c</sup> Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou, Fujian 350108, China



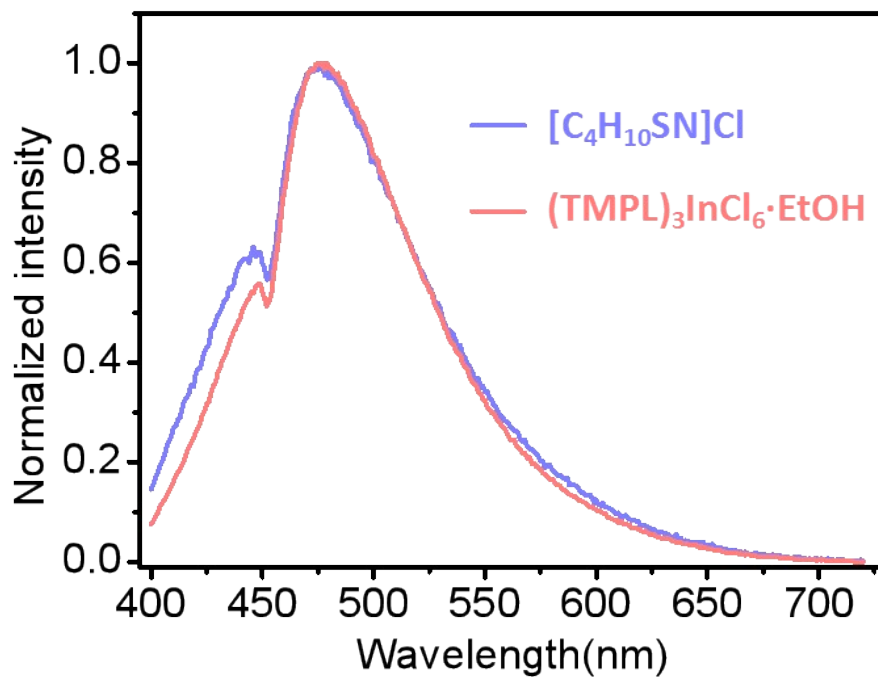
**Figure S1.** The PXRD patterns of  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH}$  and corresponding simulated one from single crystal.



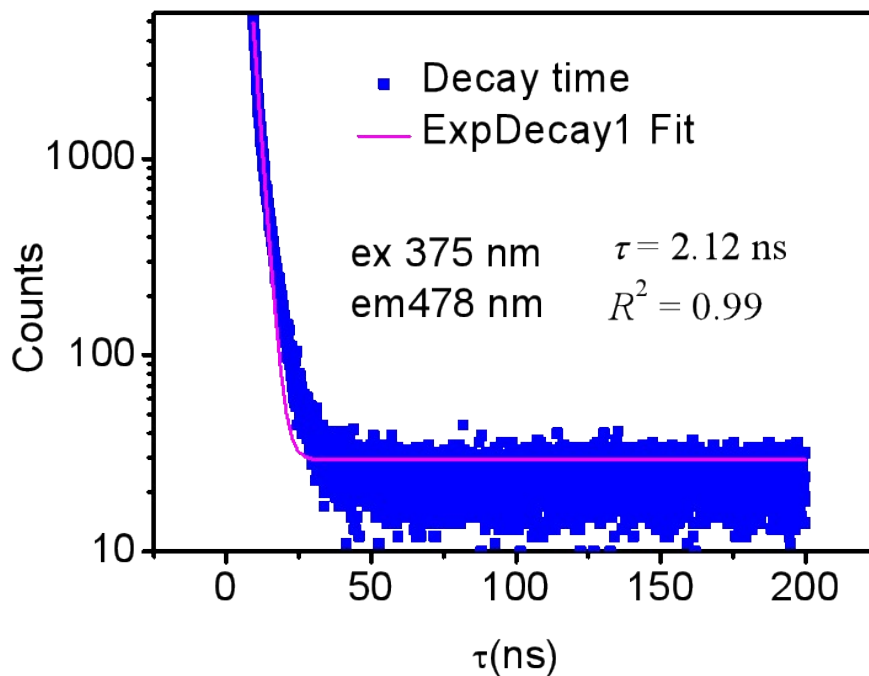
**Figure S2.** TGA curve of  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH}$  in the range of 25-1200°C.(weight loss of 6.37% refers to EtOH)



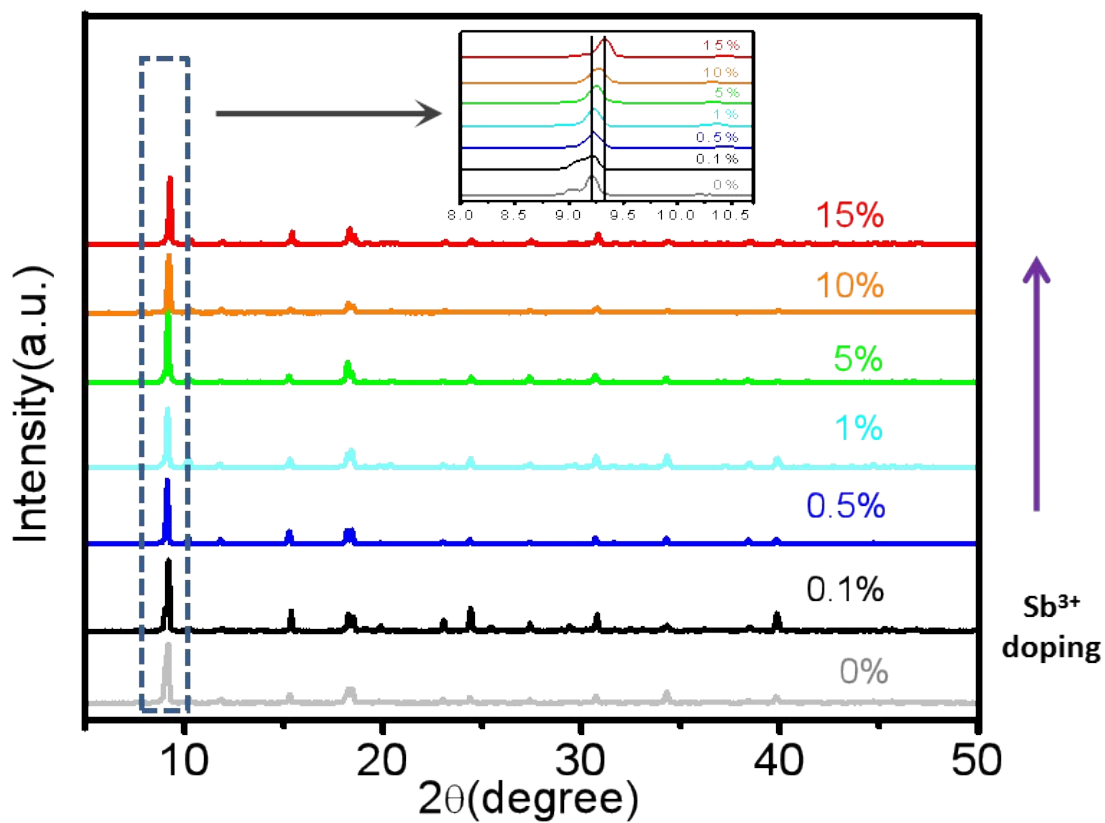
**Figure S3.** The UV-vis absorption spectra of  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH}$  at room temperature.



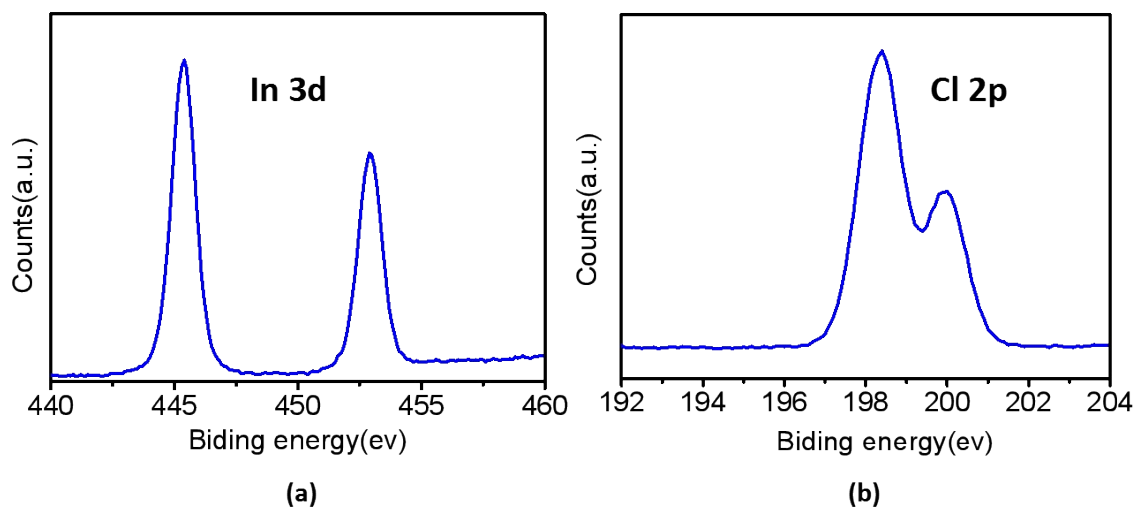
**Figure S4.** PL emission spectra of  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH}$  and  $[\text{C}_4\text{H}_{10}\text{SN}]\text{Cl}$  under excited at 340 nm.



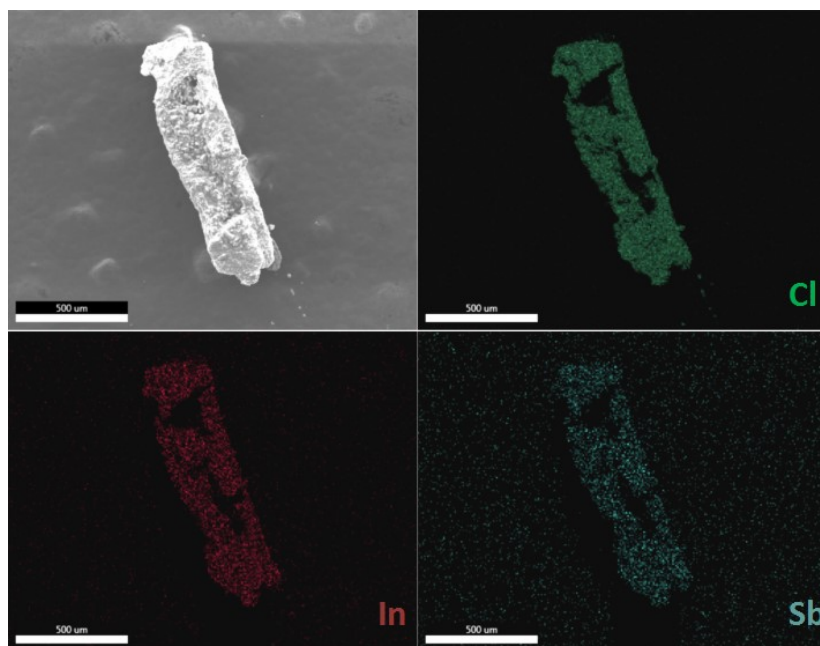
**Figure S5.** Emission decay time curve of  $[\text{C}_4\text{H}_{10}\text{SN}]\text{Cl}$  monitoring at 480 nm under excited at 375 nm.



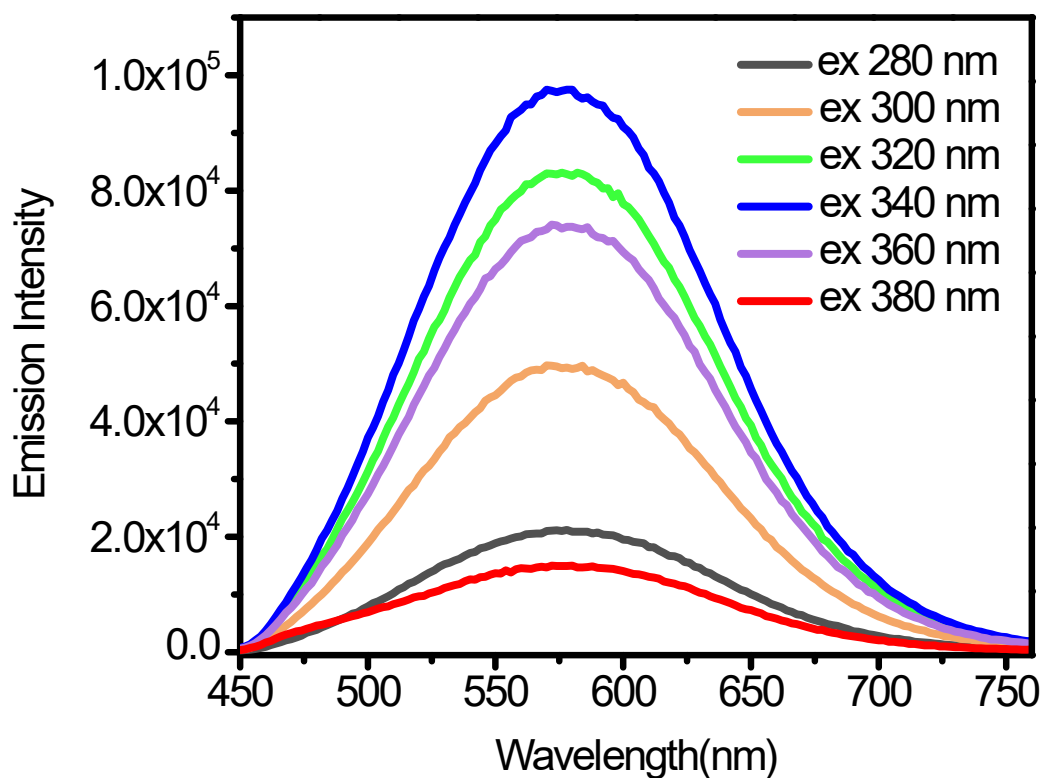
**Figure S6.** The PXRD patterns of Sb-doped  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH} : x\text{Sb}$  ( $x = 0-15\%$ ).



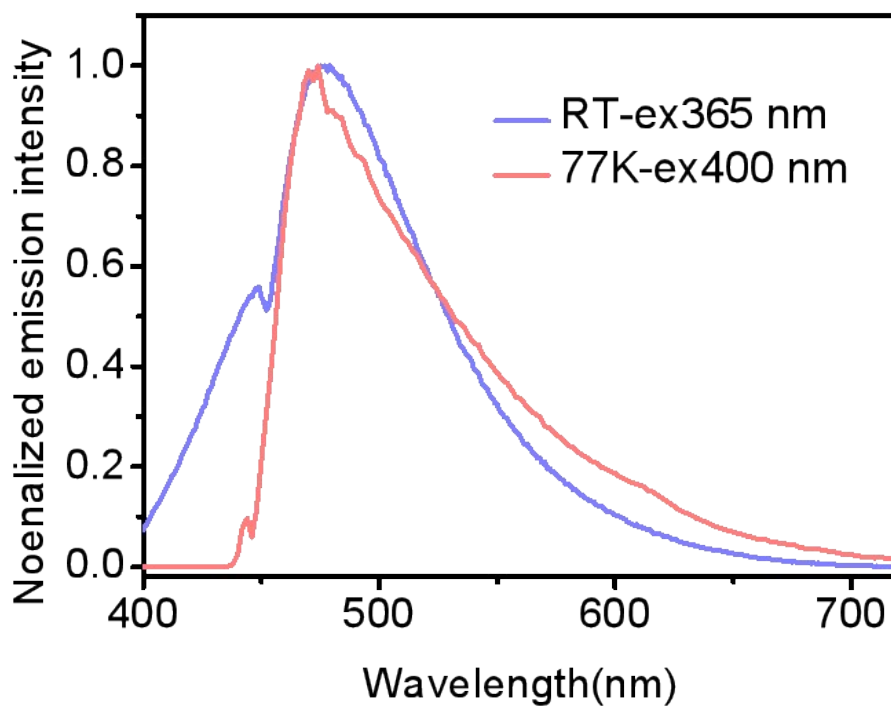
**Figure S7.** X-ray photoelectron spectroscopy (XPS) spectra in  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH} : 15\% \text{Sb}$  corresponding to In 3d and Cl 2p orbitals.



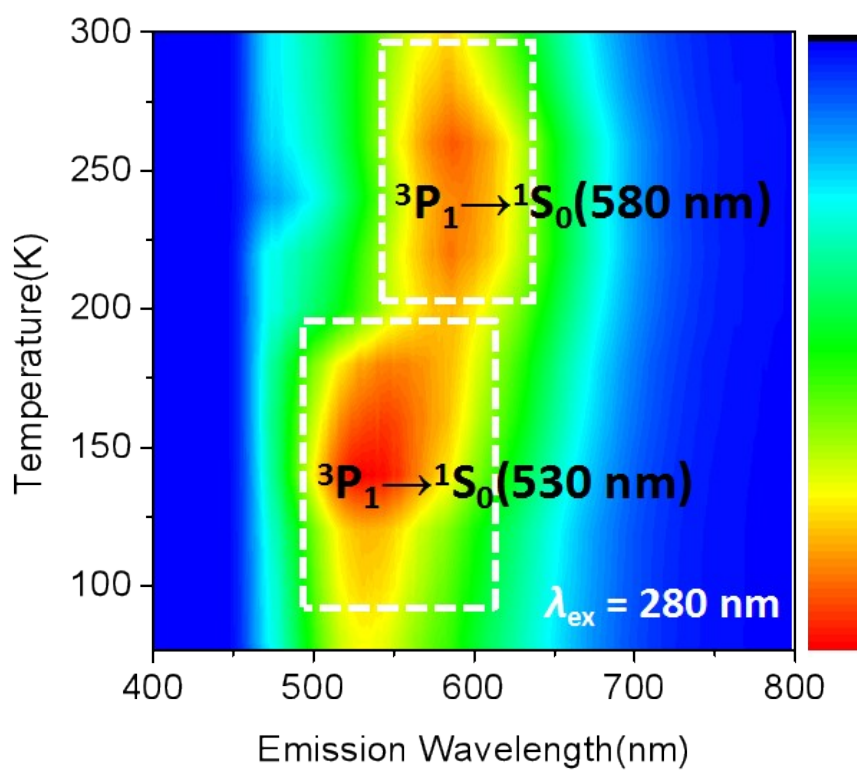
**Figure S8.** Scanning electron microscopy image (SEM) images and corresponding EDS element mapping of Cl, In, and Sb elements in  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH} : 15\% \text{Sb}$  single crystal.



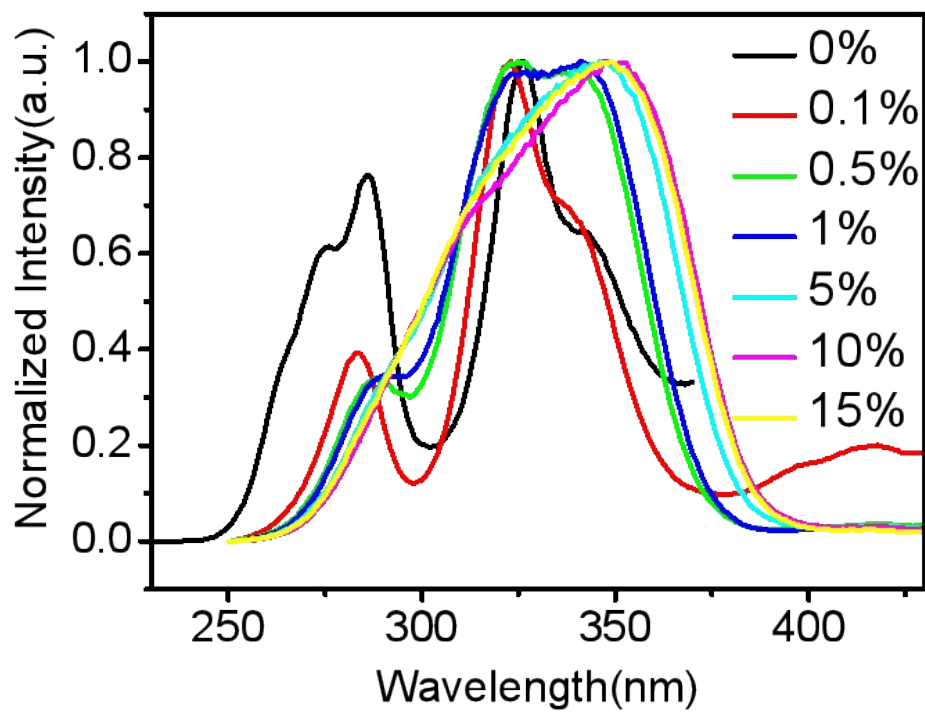
**Figure S9.** Excitation-dependent PL emission spectra of  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH} : 15\% \text{Sb}$  under various excited wavelength (280-380 nm).



**Figure S10.** Normalized PL emission spectra of  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH}$  at room temperature and low temperature (77 K).



**Figure S11.** Temperature-dependent emission spectra upon excitation at 280 nm, along with temperature change from 77-300 K.



**Figure S12.** The PLE Spectra of  $(\text{TMPL})_3\text{InCl}_6 \cdot \text{EtOH} : x\text{Sb}$  ( $x = 0-15\%$ ).

**Table S1.** Single X-Ray Diffraction Crystallographic Data of (TMPL)<sub>3</sub>InCl<sub>6</sub>·EtOH.

Compounds	(TMPL) <sub>3</sub> InCl <sub>6</sub> ·EtOH
Moiety formula	(C <sub>4</sub> H <sub>10</sub> NS) <sub>3</sub> InCl <sub>6</sub> ·C <sub>2</sub> H <sub>5</sub> OH
Sum formula	C <sub>14</sub> H <sub>36</sub> Cl <sub>6</sub> InN <sub>3</sub> OS <sub>3</sub>
Temperature/K	100
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> / Å	7.6775(6)
<i>b</i> / Å	11.6645(8)
<i>c</i> / Å	15.0912(11)
<i>α</i> / deg	83.058(3)
<i>β</i> / deg	87.367(3)
<i>γ</i> / deg	88.759(3)
volume / Å <sup>3</sup>	1339.98(17)
<i>Z</i>	2
$\rho_{\text{calc}}$ / g·cm <sup>-3</sup>	1.701
<i>F</i> (000)	696.0
Crystal size / mm <sup>3</sup>	0.72 × 0.09 × 0.09
$\mu$ / mm <sup>-1</sup>	1.721
Radiation	Mo K $\alpha$ ( $\lambda$ = 0.71073 Å)
Final <i>R</i> indexes [all data]	<i>R</i> <sub>1</sub> <sup>a</sup> =0.0518 <i>wR</i> <sub>2</sub> <sup>b</sup> =0.1474
GOF	1.077

$$(a) R_1 = \frac{\sum |F_o - F_c|}{\sum F_o}$$

$$(b) wR_2 = \frac{\sum [w(F_o^2 - F_c^2)]}{\sum [w(F_o^2)]}$$



**TableS2.** Selected bond angle (°) of (TMPL)<sub>3</sub>InCl<sub>6</sub>·EtOH.

Atom1	Atom2	Atom3	Bond angle
C12	In1	C11	90.89
C12	In1	C13	91.88
C12	In1	C11	89.11
C12	In1	C13	88.12
C11	In1	C13	89.92
C11	In1	C13	90.08
C13	In1	C11	89.92
C11	In1	C13	90.08
C11	In1	C12	89.11
C12	In1	C13	88.12
C12	In1	C13	91.88
C12	In1	C11	90.89
C16	In2	C14	90.56
C16	In2	C15	92.68
C16	In2	C14	89.44
C16	In2	C15	87.32
C15	In2	C14	91.41
C15	In2	C14	88.59
C14	In2	C15	91.41
C15	In2	C14	88.59
C14	In2	C16	90.56
C15	In2	C16	87.32
C16	In2	C14	89.44
C16	In2	C15	92.68

**Table S3.** Selected bond length (Å) of (TMPL)<sub>3</sub>InCl<sub>6</sub>·EtOH.

Atom1	Atom2	Bond length
C11	In1	2.505
C13	In1	2.523
C12	In1	2.540
C11	In1	2.505
C13	In1	2.523
C12	In1	2.540
C14	In2	2.532
C16	In2	2.520
In2	C15	2.516
In2	C16	2.520
In2	C14	2.532
In2	C15	2.516

**Table S4.** Photophysical parameter of (TMPL)<sub>3</sub>InCl<sub>6</sub>·EtOH and (TMPL)<sub>3</sub>InCl<sub>6</sub>·EtOH:15%Sb.

	(TMPL) <sub>3</sub> InCl <sub>6</sub> ·EtOH	(TMPL) <sub>3</sub> InCl <sub>6</sub> ·EtOH:15%Sb
$\lambda_{em}^a$ /nm	478	580
$\tau^b$ /μs	$2.95 \times 10^{-3}$	2.18
$\Phi_{em}^c$ /%	1.73	85.35

<sup>a,c</sup> Excitation at 350 nm. <sup>b</sup> Excitation at 375 nm with EPL-375 picosecond pulsed diode laser.