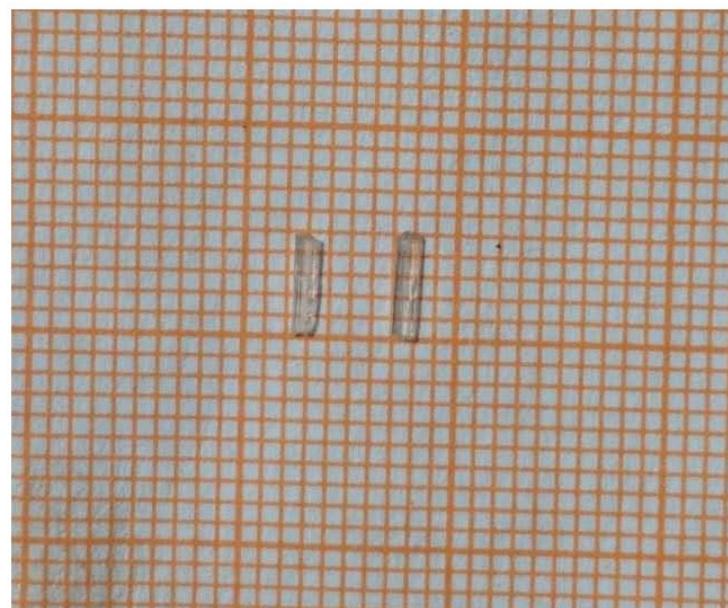


# A Lead-free Semiconducting Hybrid with Ultra-high Color Rendering Index White Light-emission

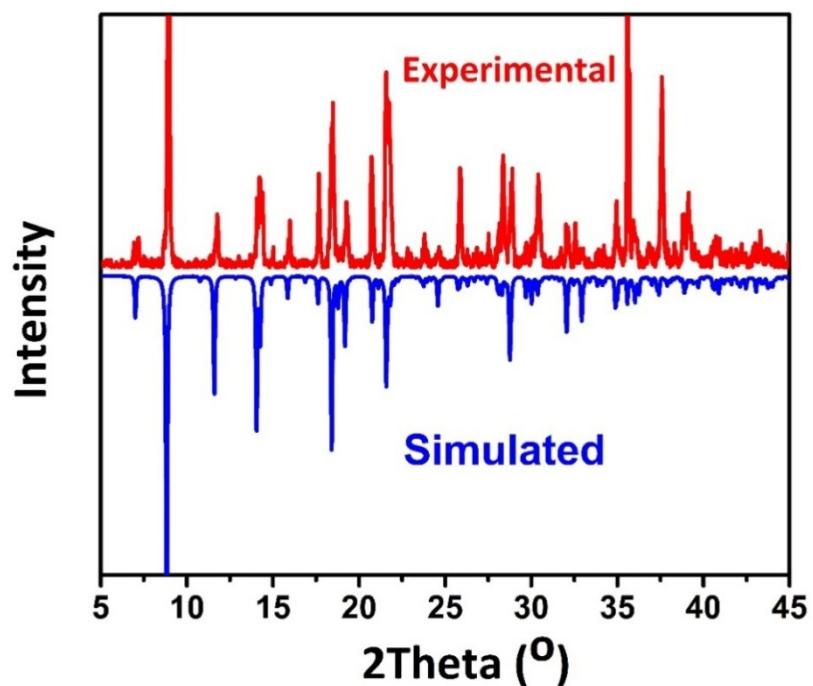
Asma Khan,<sup>a,b</sup> Aurang Zeb,<sup>a,b</sup> Lina Li,<sup>a</sup> Weichuan Zhang,<sup>a</sup> Zhihua Sun,<sup>a</sup> Yuyin Wang,<sup>a,b</sup> and Junhua Luo,<sup>\*,a</sup>

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

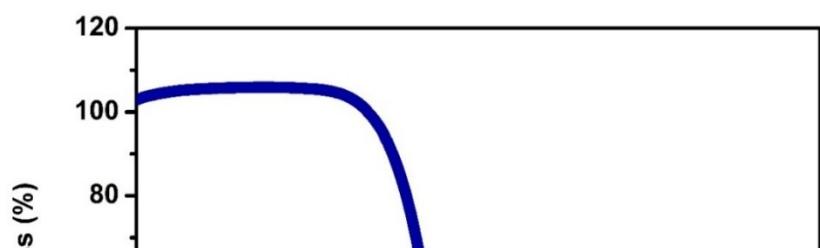
<sup>b</sup> University of Chinese Academy of Sciences, Chinese Academy of Sciences, Beijing 100039, P. R. China



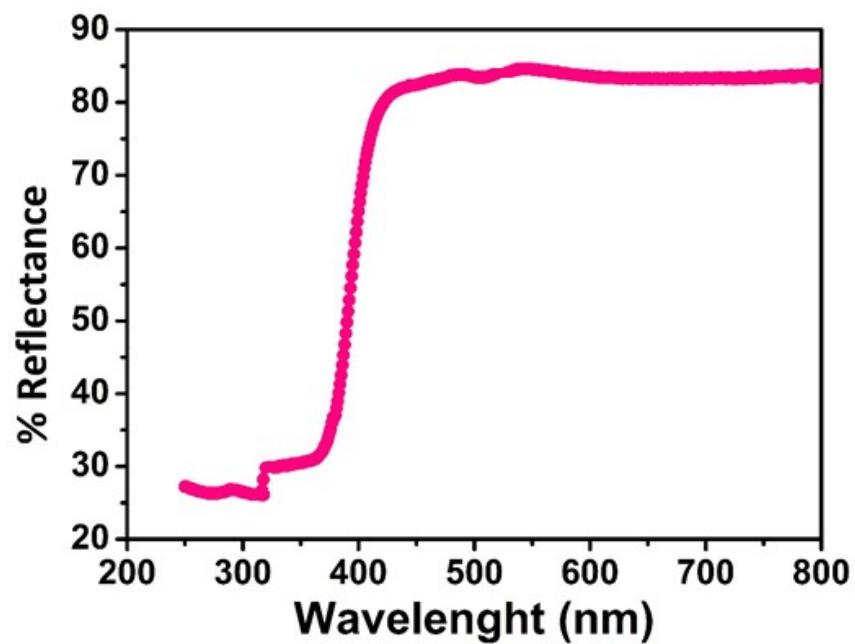
**Figure S1.** Colorless needle like Single crystal of **4-MPSC**



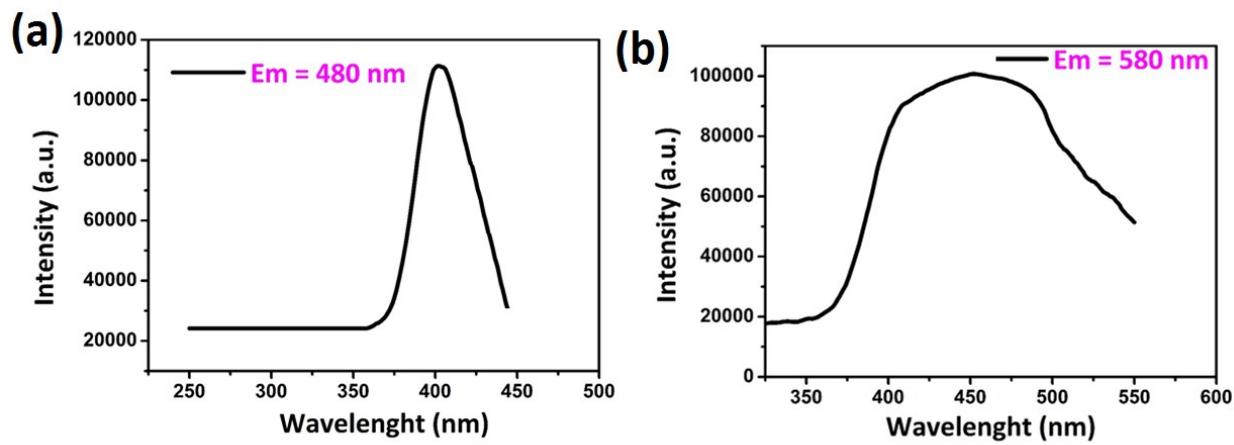
**Figure S2.** PXRD patterns of **4-MPSC**.



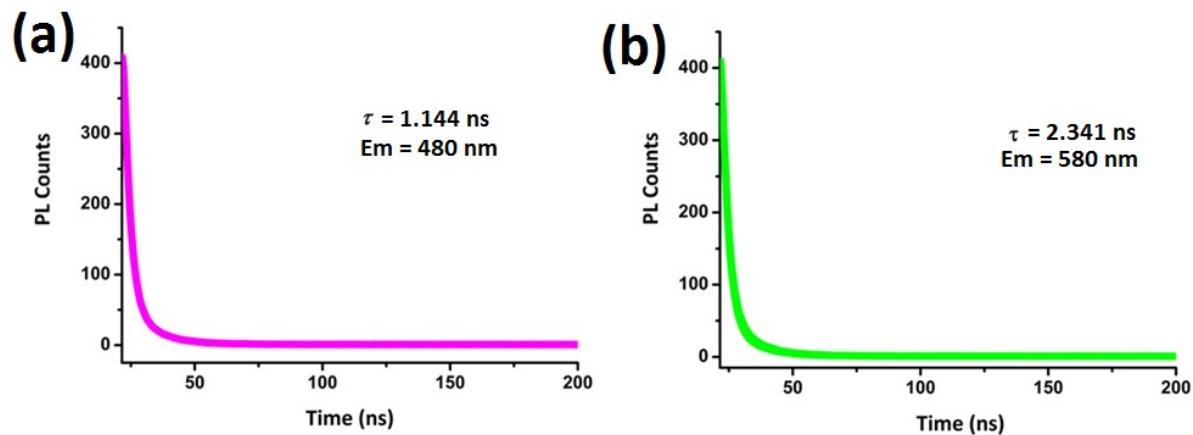
**Figure S3.** TG curve of 4-MPSC.



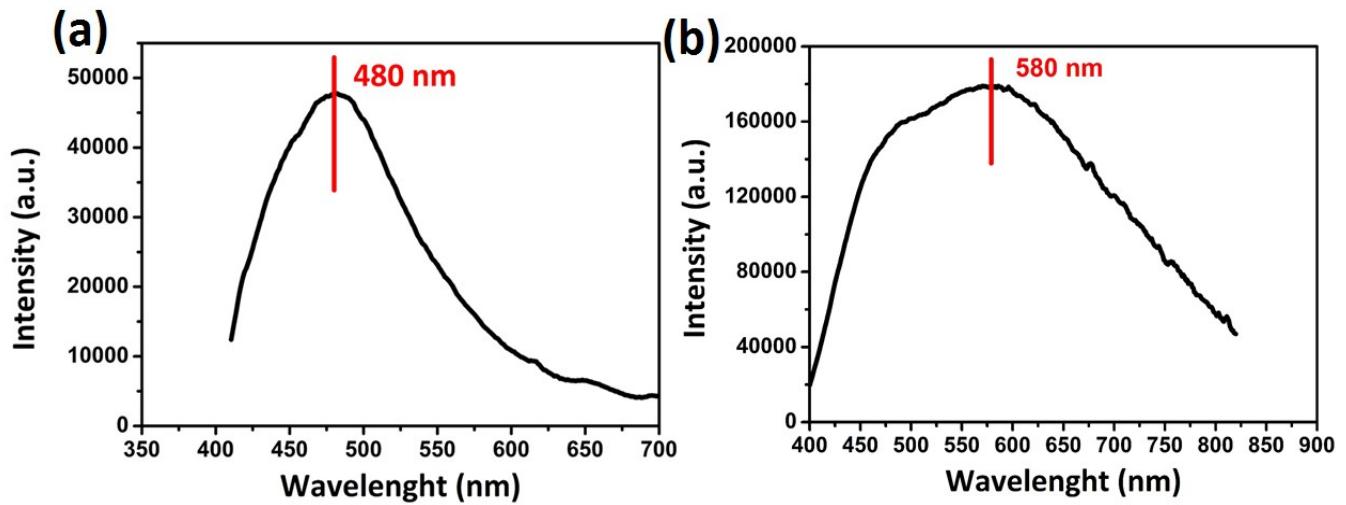
**Figure S4.** UV-vis diffuse reflectance spectroscopy of 4-MPSC.



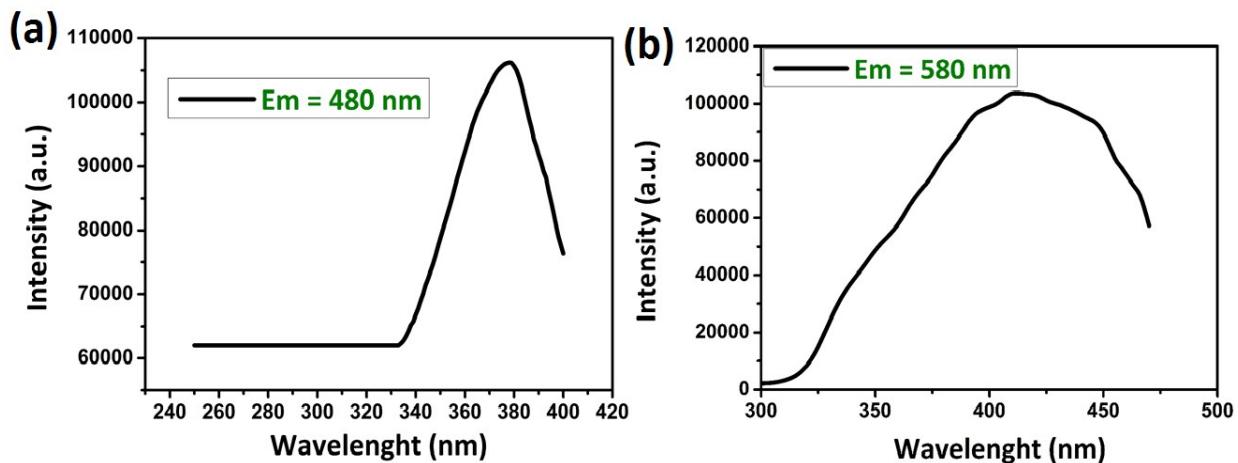
**Figure S5.**(a) Excitation spectrum of **4-MPSC** at 480 nm and (b) 580 nm.



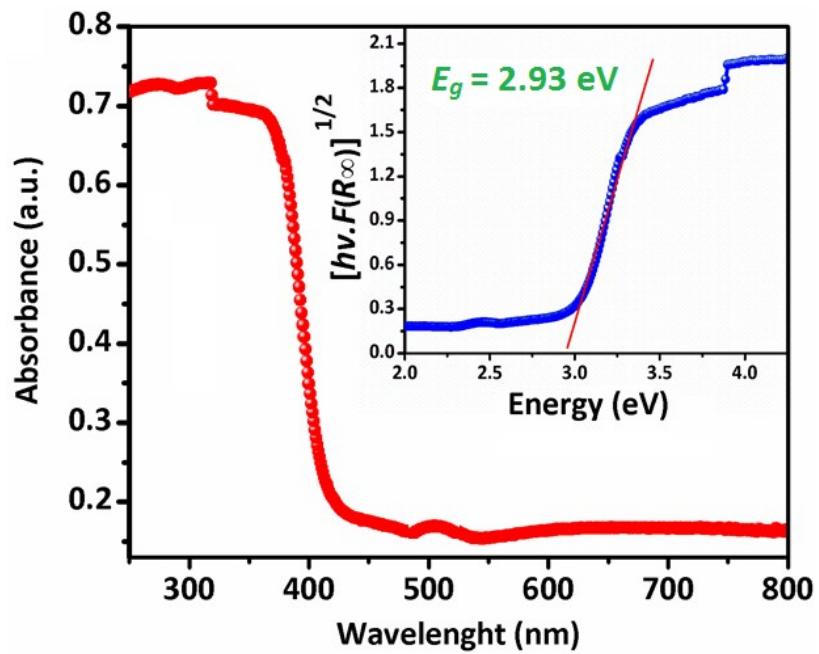
**Figure S6.** Luminescence decay data of **4-MPSC** at (a) 480 nm (b) and 580 nm.



**Figure S7.** Emission spectrum of (a)  $[4\text{-methyl Piperidium}]^+\text{Cl}^-$  and (b)  $\text{SbCl}_5$ .



**Figure S8.** Excitation spectrum of (a)  $[4\text{-methyl Piperidium}]^+\text{Cl}^-$  and (b)  $\text{SbCl}_5$ .



**Figure S9.** UV-vis absorption spectra of **4-MPSC**, inset: the optical bandgap deduced from the *Tauc* plot.

**Table S1.** Crystallographic data and structure refinement of **4-MPSC**.

Formula	C <sub>12</sub> H <sub>28</sub> Cl <sub>5</sub> N <sub>2</sub> Sb
Formula weight (g/mol)	499.36
Temperature (K)	215
Crystal system	Monoclinic
Space group	P 21/c
a (Å)	12.9832(2)
b (Å)	16.4632(2)
c (Å)	9.72240(10)
α (deg)	90
θ (deg)	103.823(1)
γ (deg)	90
V (Å <sup>3</sup> )	2017.93
Z	4
R-Factor (%)	5.69
D <sub>cald</sub> (g/cm <sup>3</sup> )	1.677
F (000)	1000.0
Completeness (%)	99.2
GOF ( <i>F</i> <sup>2</sup> )	1.105
R1 (on <i>F</i> <sub>o</sub> <sup>2</sup> , <i>I</i> > 2σ( <i>I</i> ))	0.0570
wR2 (on <i>F</i> <sub>o</sub> <sup>2</sup> , <i>I</i> > 2σ( <i>I</i> ))	0.1400

<sup>a</sup>*R*<sub>1</sub> = Σ ||*F*<sub>0</sub>|| - ||*F*<sub>c</sub>|| / Σ ||*F*<sub>0</sub>||, w*R*2 = [Σ [*ω*(*F*<sub>0</sub><sup>2</sup> - *F*<sub>c</sub><sup>2</sup>)<sup>2</sup>] / Σ [*ω*(*F*<sub>0</sub><sup>2</sup>)<sup>2</sup>]]<sup>1/2</sup>

**Table S2.** Selected bond length (Å).

Bond	[Å]
Sb2-Cl1	2.608(1)
Sb2-Cl2	2.482(1)
Sb2-Cl3	3.199(1)
Sb2-Cl4	2.637(9)
Sb2-Cl5	2.865(1)
Sb2-Cl6	2.424(1)

**Table S3.** The length of H-bonds of **4-MPSC**

Bond	[Å]
(N <sub>10</sub> - H <sub>10A</sub> …Cl <sub>5</sub> )	3.273 Å
(N <sub>10</sub> - H <sub>10B</sub> …Cl <sub>3</sub> )	3.293 Å