Supporting Information

Bulk assembly of 0D organic antimony chloride hybrid with highly efficient orange dual-emission by self-trapped states

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Table S1. Crystal data and structure refinement for $(TPA)_2SbCl_5$ single crystal.

Empirical formula	$C_{24}H_{56}Cl_5N_2Sb$
Formula weight	671.70
Temperature/K	170.0(3)
Crystal system	triclinic
Space group	P-1
a/Å	10.6100(2)
b/Å	10.7418(2)
c/Å	16.2363(3)
α/°	76.000(2)
β/°	74.827(2)
γ/°	72.614(2)
Volume/Å^3	1677.22(6)
Z	2
ρ_{calc}g/cm^3	1.330
μ/mm^{-1}	1.235
F(000)	700.0
Crystal size/mm^3	0.22 × 0.21 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.038 to 61.946
Index ranges	$-14 \le h \le 14$, $-11 \le k \le 15$, $-23 \le l \le 23$
Reflections collected	25968
Independent reflections	8994 [R_{int} = 0.0289, R_{sigma} = 0.0311]
Data/restraints/parameters	8994/0/297
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0230, wR_2 = 0.0530
Final R indexes [all data]	R_1 = 0.0255, wR_2 = 0.0543
Largest diff. peak/hole / e Å^{-3}	0.42/-0.43

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $(TPA)_2SbCl_5$ single crystal. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sb1	6370.9(2)	3778.0(2)	7769.5(2)	22.38(3)
Cl1	7993.3(4)	5246.0(4)	6754.3(2)	30.14(8)
Cl2	4216.4(4)	5738.0(4)	7668.9(3)	42.06(10)
Cl3	6264.2(4)	3265.6(5)	6460.6(2)	36.97(9)
Cl4	4831.5(4)	2227.0(4)	8562.7(2)	30.90(8)
Cl5	8433.2(4)	1748.5(4)	7951.0(3)	38.11(9)
N1	6797.0(14)	7895.7(12)	8546.6(8)	27.2(3)
C1	6884.6(18)	6417.4(14)	8793.2(10)	29.6(3)
C2	7041.4(19)	5771.4(16)	9709.0(10)	34.0(3)
C3	7028.1(19)	4317.2(16)	9858.8(11)	36.3(4)
C4	7917.1(17)	8234.3(16)	8795.6(10)	32.4(3)
C5	9335.8(19)	7587(2)	8377.1(14)	45.8(4)
C6	10341(2)	7947(3)	8735.8(16)	60.9(6)
C7	5479.7(17)	8688.1(15)	9017.8(10)	30.2(3)
C8	4204.3(19)	8692.9(19)	8766.0(13)	41.3(4)
C9	2990(2)	9378(2)	9375.7(15)	53.5(5)
C10	6898.1(19)	8234.3(15)	7573.2(9)	31.6(3)
C11	6862(2)	9669.1(16)	7166.6(10)	36.9(4)
C12	7108(3)	9806.3(19)	6195.1(11)	56.6(6)
N2	2235.3(12)	3234.2(13)	6265.2(8)	26.6(3)
C13	2320.4(16)	3289.6(17)	7175.0(9)	30.8(3)
C14	980.3(17)	3760.5(19)	7764.8(10)	35.6(4)
C15	1208.5(19)	3759(2)	8649.6(11)	45.1(4)
C16	1491.2(16)	4561.1(16)	5823.9(10)	29.6(3)
C17	2001(2)	5748.2(18)	5798.3(12)	42.4(4)
C18	1049(2)	6987(2)	5412.1(16)	58.3(6)
C19	1454.6(17)	2246.6(17)	6289.9(11)	34.2(3)
C20	2018(2)	829(2)	6703.9(15)	52.9(5)
C21	1340(3)	-80(2)	6487.5(17)	66.2(7)
C22	3674.6(15)	2842.1(17)	5767.5(10)	30.9(3)
C23	3846.3(19)	2593(2)	4868.0(12)	50.5(5)

C24	5288.5(19)	2165(2)	4444.9(12)	48.6(5)

Table S3. Bond lengths for $(TPA)_2SbCl_5$ single crystal.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Sb1	Cl1	2.6543(4)	C10	C11	1.516(2)
Sb1	Cl2	2.6150(4)	C11	C12	1.508(2)
Sb1	Cl3	2.3582(4)	N2	C13	1.5196(19)
Sb1	Cl4	2.5669(4)	N2	C16	1.516(2)
Sb1	Cl5	2.6082(4)	N2	C19	1.517(2)
N1	C1	1.5212(19)	N2	C22	1.5155(19)
N1	C4	1.513(2)	C13	C14	1.512(2)
N1	C7	1.519(2)	C14	C15	1.518(2)
N1	C10	1.5161(18)	C16	C17	1.515(2)
C1	C2	1.510(2)	C17	C18	1.519(3)
C2	C3	1.525(2)	C19	C20	1.517(3)
C4	C5	1.509(3)	C20	C21	1.520(3)
C5	C6	1.518(3)	C22	C23	1.503(2)
C7	C8	1.511(2)	C23	C24	1.485(3)
C8	C9	1.516(3)			

Table S4. Bond angles for $(TPA)_2SbCl_5$ single crystal.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	Sb1	Cl1	92.716(13)	C4	C5	C6	109.67(18)
Cl3	Sb1	Cl1	84.465(13)	C8	C7	N1	116.72(13)
Cl3	Sb1	Cl2	90.301(16)	C7	C8	C9	109.34(16)
Cl3	Sb1	Cl4	87.676(14)	N1	C10	C11	115.65(12)
Cl3	Sb1	Cl5	90.974(16)	C12	C11	C10	108.78(14)
Cl4	Sb1	Cl1	172.012(12)	C16	N2	C13	111.48(12)
Cl4	Sb1	Cl2	88.744(14)	C16	N2	C19	106.28(12)
Cl4	Sb1	Cl5	88.067(13)	C19	N2	C13	110.83(12)
Cl5	Sb1	Cl1	90.636(13)	C22	N2	C13	106.55(11)
Cl5	Sb1	Cl2	176.514(14)	C22	N2	C16	110.44(12)
C4	N1	C1	111.53(12)	C22	N2	C19	111.33(12)
C4	N1	C7	106.46(11)	C14	C13	N2	115.03(12)
C4	N1	C10	111.01(12)	C13	C14	C15	109.60(14)
C7	N1	C1	110.99(12)	C17	C16	N2	116.41(13)
C10	N1	C1	105.75(11)	C16	C17	C18	108.31(16)
C10	N1	C7	111.19(12)	C20	C19	N2	115.99(15)
C2	C1	N1	116.63(12)	C19	C20	C21	109.28(19)
C1	C2	C3	109.55(13)	C23	C22	N2	116.18(13)
C5	C4	N1	115.92(14)	C24	C23	C22	112.29(15)
Cl2	Sb1	Cl1	92.716(13)	C4	C5	C6	109.67(18)

Table S4. Comparison of room temperature key photophysical parameters of $(TPA)_2SbCl_5$ with recently reported orange-emitting quantum dots (QDs) or phosphors.

Components	Emission peak (nm)	PLQY(%)	Lifetime (μs)	Pros and cons	Ref.
$(TPA)_2SbCl_5$	610	95.3	5.3	stable, low-toxic, high PLQY	This work
$(OAm)_2SnBr_4$	628	60	4.3	easily oxidized	[1]
$(DAO)Sn_2I_6$ film	634	36	1.114	Water-Stable/low PLQY	[2]
$(PMA)_3InBr_6$	610	35	～1.25	low-toxic/low PLQY	[3]
$(R/S\text{-}MBA)_4Cu_4I_4$	630	52.8/59.7	～15.4/14.9	easily oxidized	[4]
$C_4H_{14}N_2MnBr_4$	516, 623	10.39	3.6, 183.2	low-toxic/low PLQY	[5]
$(C_9NH_{20})_2SbCl_5$	590	98	4.2	low-toxic, high PLQY	[6]
$(C_6N_2H_{16})SbCl_5$	613	25.3	1.06	low-toxic/low PLQY	[7]
$(C_6N_2H_{16})SbCl_5{\cdot}H_2O$	620	39.6	1.22	low-toxic/low PLQY	[7]
$Cs_2SnCl_6:Sb^{3+}$ NCs	438 and 615	8.25	-	low-toxic/low PLQY	[8]
$CsPb_{0.835}Mn_{0.165}Cl_3$ QDs	～397 and 615	34	847	Toxic and low PLQY	[9]
$Cs_2AgInCl_6:Mn^{2+}$ NCs	620	16	μs level	low-toxic/low PLQY	[10]
$Cs_4MnBi_2Cl_{12}$	610	25.7	144	low-toxic/low PLQY	[11]

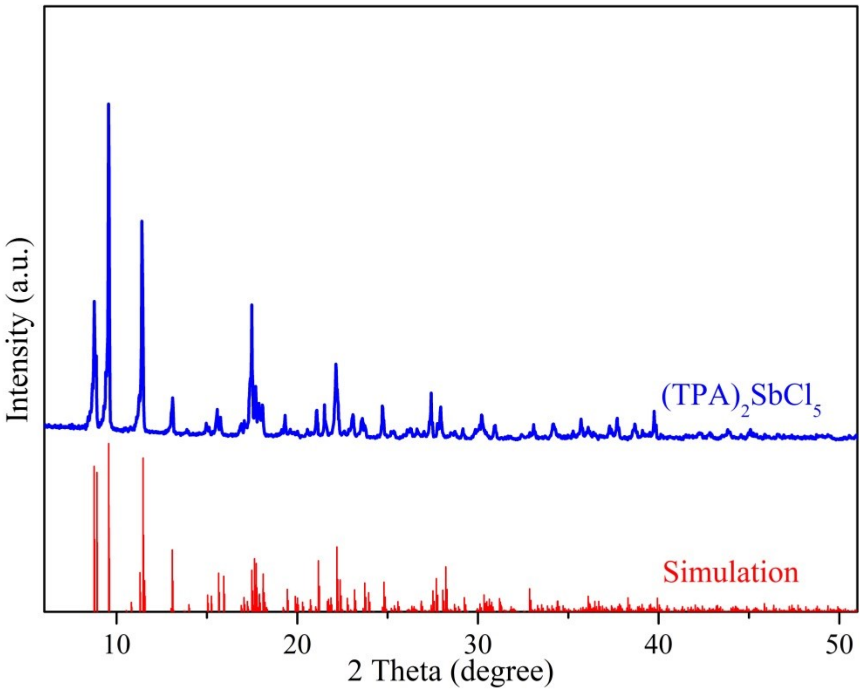

Figure S1. Experimental and simulated PXRD patterns of $(TPA)_2SbCl_5$.

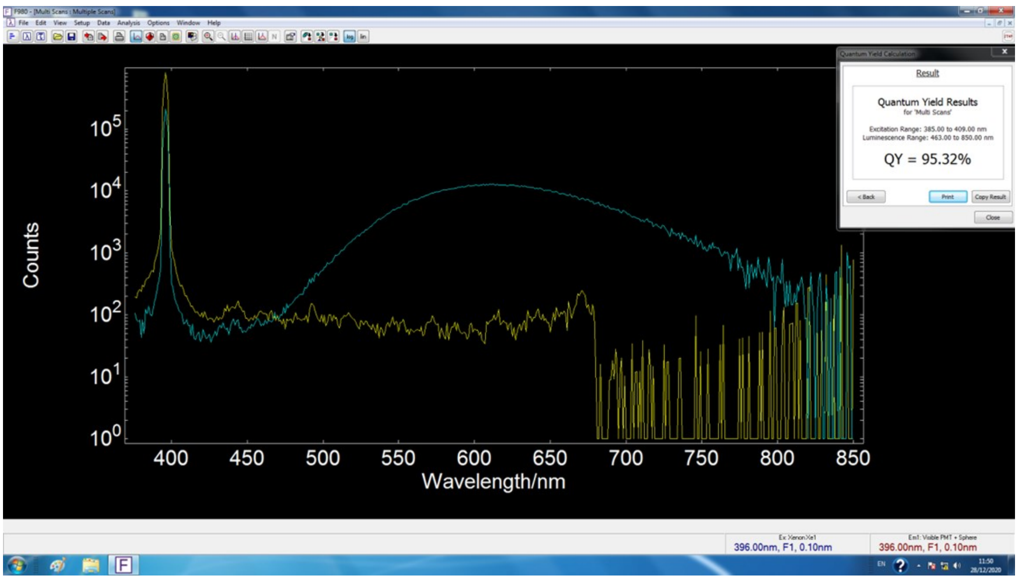

Figure S2. Absolute photoluminescence quantum yield measurement of the $(TPA)_2SbCl_5$ SCs.

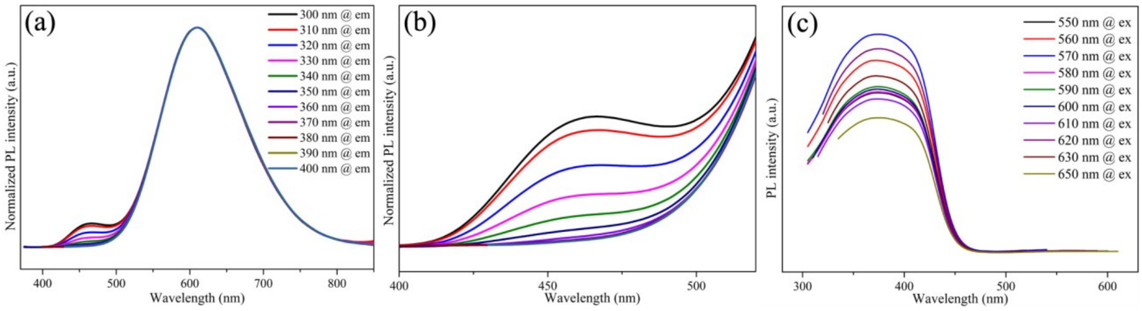

Figure S3. (a) Excitation-wavelength dependent photoluminescence (PL) spectra. (b) The Magnified area of the PL spectra in the wavelength range of 400-520 nm. (c) Emission-wavelength-dependent photoluminescence excitation (PLE) spectra of $(TPA)_2SbCl_5$ SCs at room temperature.

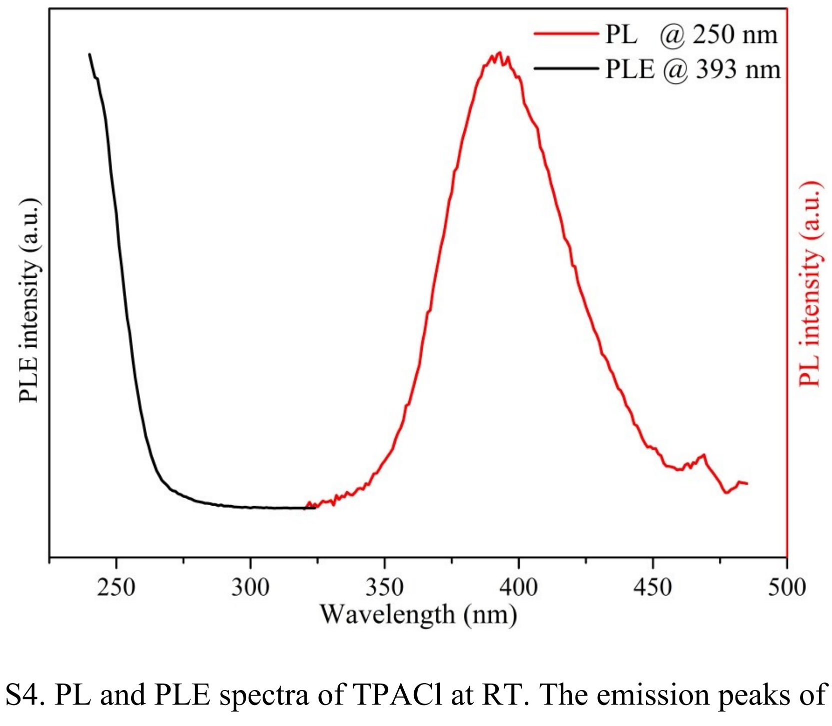

Figure S4. PL and PLE spectra of TPACl at RT. The emission peaks of TPACl appeared at around 393 nm.

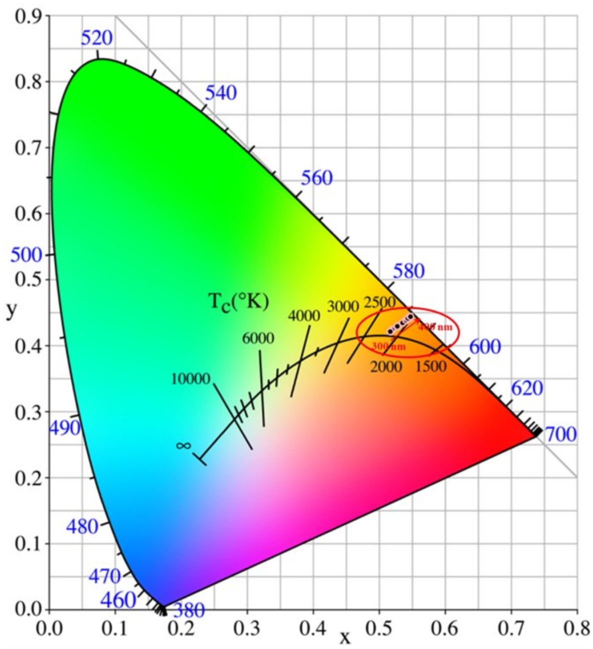

Figure S5. The Commission Internationale de l'Eclairage (CIE) chromaticity diagram of $(TPA)_2SbCl_5$ were calculated to evaluate the emission change quantitively under different excitation wavelength from 300 to 400 nm.

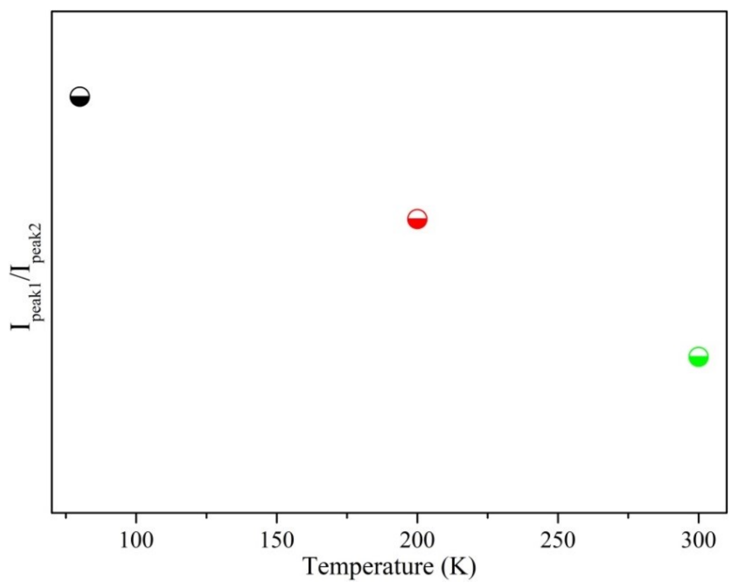

Figure S6. I_{Peak1}/I_{Peak2} extracted from low temperature-dependent PL spectra.

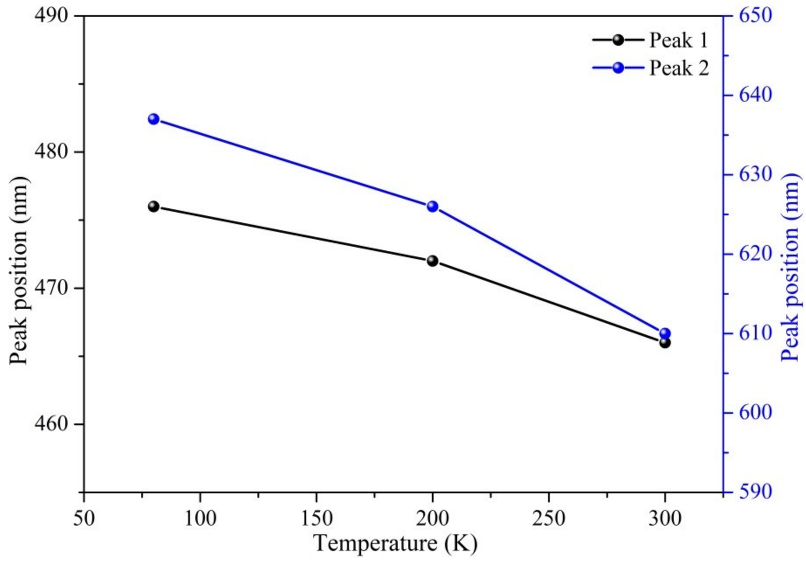

Figure S7. The PL peak position of$(TPA)_2SbCl_5$ SCs as a function of low temperature.

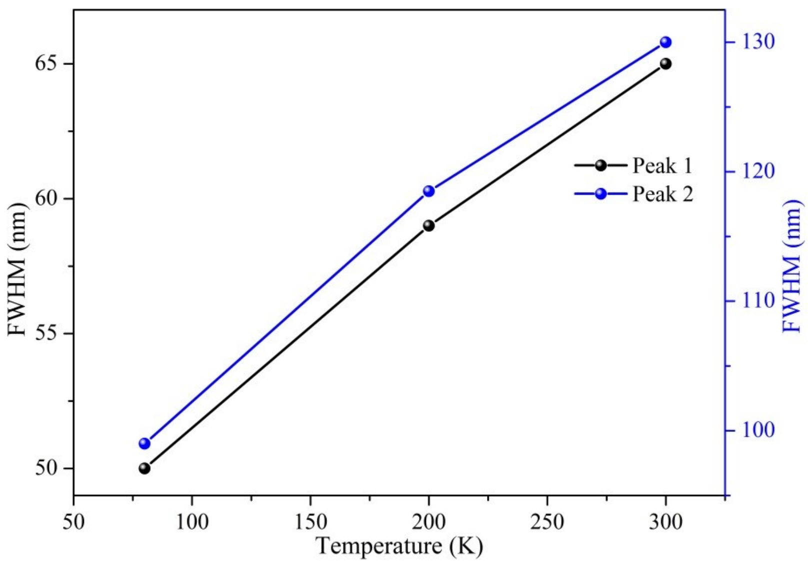

Figure S8. The FWHM of$(TPA)_2SbCl_5$ SCs as a function of low temperature.

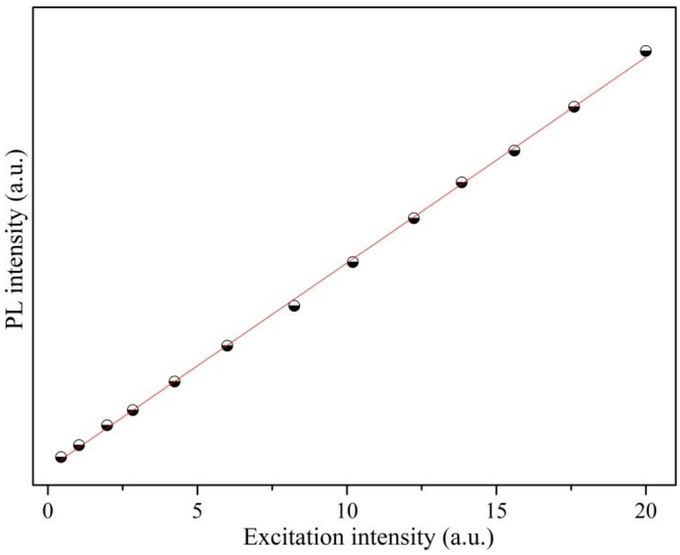

Figure S9. The PL intensity versus excitation power for $(TPA)_2SbCl_5$ SCs excited by 405 nm laser at room temperature.

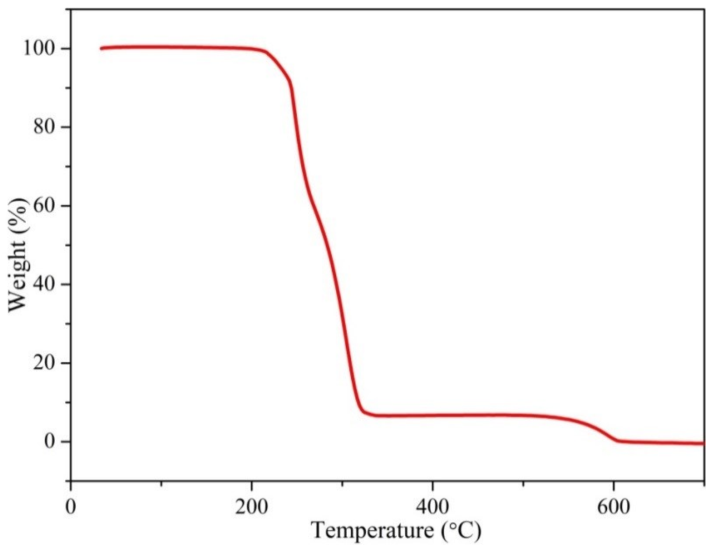

Figure S10. TG curve of $(TPA)_2SbCl_5$ powders.

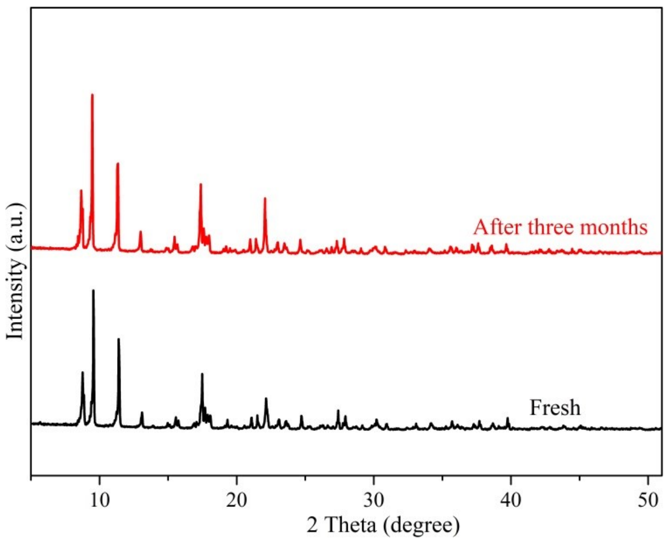

Figure S11. PXRD patterns of $(TPA)_2SbCl_5$ before and after exposure to atmospheric environment (～50 % relative humidity) for three month.

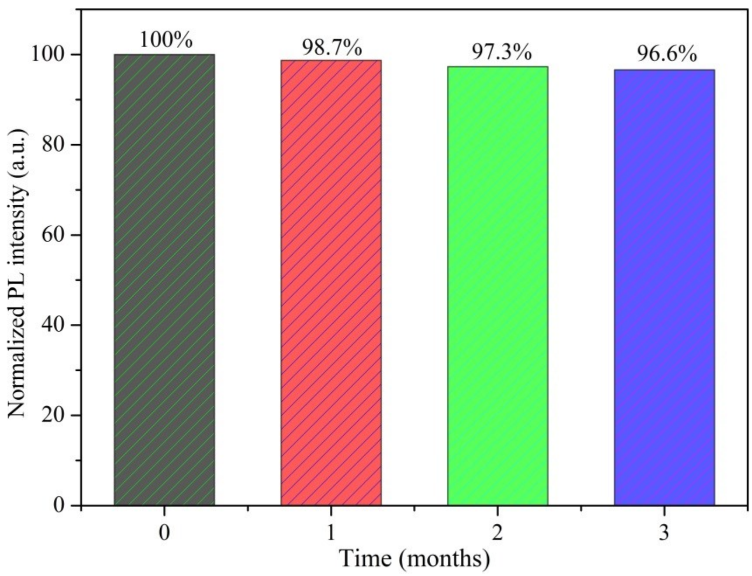

Figure S12. The PL intensity of $(TPA)_2SbCl_5$ SCs at different times (～50 % relative humidity) within three months.

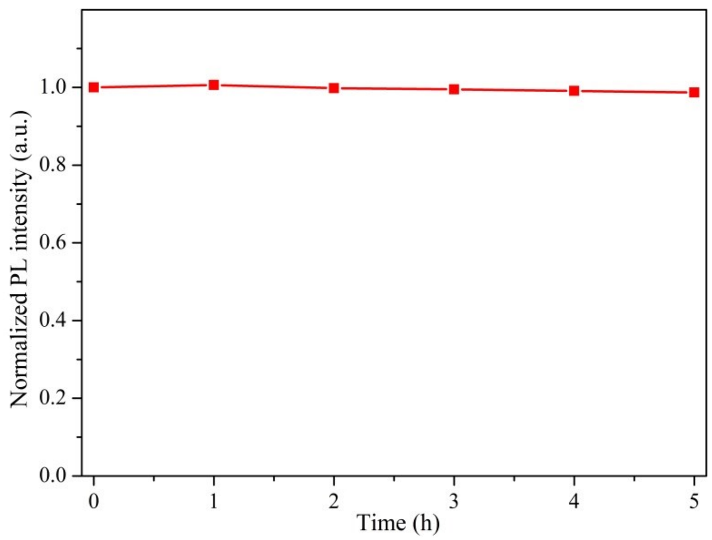

Figure S13. Long-term stability of $(TPA)_2SbCl_5$ SCs under a 325 nm UV lamp within 5 h.

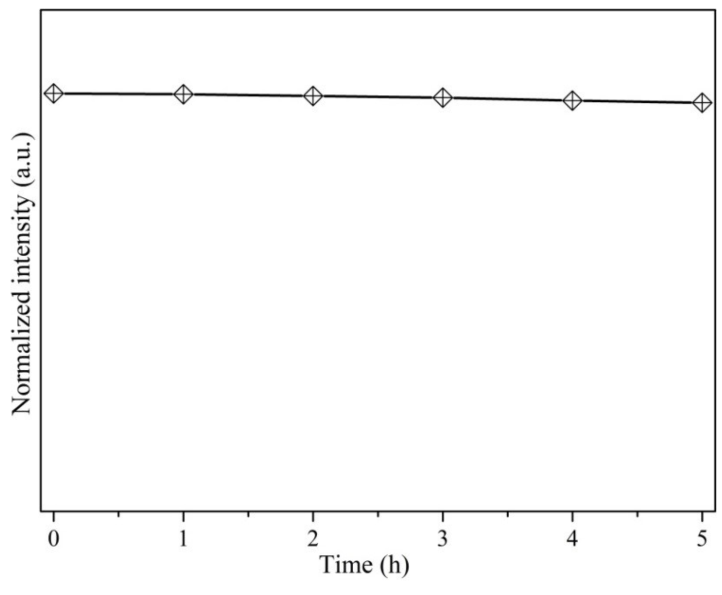

Figure S14. Long-term stability of WLED when it operates for 5 h.

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