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Antimony and Bismuth Cooperation to Enhance the Broad Yellow Photoluminescence of Zero-Dimensional Hybrid Halide

Jindong Cao,[†] Jiawei Lin,[†] Kunjie Liu,[†] Yan, Xiong,[hu] Na Wang,[†] Shihui He,[†] Xusheng Zhang,[†] Zhongnan Guo,[†] Xin Chen,[⊥] Jing Zhao,[†,*] and Quanlin Liu[†]

[†] School of Materials Sciences and Engineering & School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing 100083, China.

[hu] The State Key Laboratory of HVDC (Electric Power Research Institute, China Southern Power Grid), Guangzhou 510663, Guangdong Province, China.

[⊥] Beijing Advanced Innovation Center for Materials Genome Engineering, Institute of Solid State Chemistry, University of Science and Technology Beijing, Beijing 100083, China.

[*]**Corresponding Author**：

E-mail: jingzhao@ustb.edu.cn

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Label	x	y	z	Occupancy	U_{eq}*
Cl(1)	0(2)	-256(2)	4337(1)	1	43(1)
Cl(2)	-235(2)	-475(2)	3029(1)	1	41(1)
Cl(3)	2725(2)	-1789(2)	3768(1)	1	40(1)
Cl(4)	3287(2)	332(2)	2977(1)	1	35(1)
Cl(5)	3736(2)	870(2)	4256(1)	1	41(1)
Cl(6)	627(2)	2064(2)	3620(1)	1	37(1)
Sb(34)	1620(1)	135(1)	3694(1)	0.403(4)	22(1)
Bi(2)	1620(1)	135(1)	3694(1)	0.597(4)	22(1)
Cl(7)	6694(2)	3070(2)	3833(1)	1	42(1)
Cl(8)	6563(2)	5504(2)	4516(1)	1	49(1)
Cl(9)	8771(2)	7010(2)	3810(1)	1	37(1)
Cl(10)	10131(2)	4768(2)	4385(1)	1	39(1)
Cl(11)	9217(2)	4680(2)	3037(1)	1	39(1)
Cl(12)	5857(2)	5701(2)	3236(1)	1	44(1)
Sb(35)	7928(1)	5117(1)	3795(1)	0.509(4)	24(1)
Bi(1)	7928(1)	5117(1)	3795(1)	0.491(4)	24(1)
O(36)	4521(10)	1876(6)	2088(3)	1	77(3)
N(13)	10622(7)	2879(5)	5072(2)	1	35(2)
N(14)	6925(6)	2402(5)	4871(2)	1	32(2)
C(19)	11795(8)	2318(7)	4919(3)	1	40(2)
C(20)	9371(8)	2385(6)	4874(3)	1	33(2)
C(21)	8191(8)	2863(7)	5085(3)	1	34(2)
C(22)	6854(9)	1250(7)	4936(3)	1	40(2)
C(23)	5763(8)	2908(7)	5057(3)	1	39(2)
N(15)	7791(7)	1577(6)	3095(3)	1	41(2)
N(16)	5927(8)	-629(6)	3597(3)	1	41(2)
C(24)	6154(10)	-1117(7)	4071(3)	1	43(2)
C(25)	6206(10)	-1392(7)	3236(3)	1	44(2)
C(26)	6768(9)	334(7)	3586(3)	1	40(2)
C(27)	6661(9)	864(7)	3120(3)	1	39(2)
C(28)	7738(10)	2199(8)	2666(3)	1	47(2)
N(17)	3505(7)	4566(6)	3648(3)	1	40(2)
N(18)	2906(7)	3135(6)	2503(2)	1	38(2)
C(29)	1577(9)	2643(7)	2476(3)	1	41(2)
C(30)	3529(8)	3342(7)	2980(3)	1	40(2)

C(31)	2808(9)	4237(7)	3193(3)	1	39(2)
C(32)	3387(9)	3773(7)	4018(3)	1	43(2)
C(33)	2975(11)	5594(8)	3787(4)	1	53(3)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Anisotropic displacement parameters ($Å^2×10^3$) for $(C_5H_{16}N_2)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}·H_2O$ at 150.0 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	47(2)	48(2)	34(2)	1(1)	9(1)	4(1)
Cl(2)	34(2)	48(2)	39(2)	4(1)	-2(1)	-9(1)
Cl(3)	53(2)	31(1)	34(2)	5(1)	2(1)	1(1)
Cl(4)	35(1)	37(2)	33(1)	-1(1)	5(1)	2(1)
Cl(5)	38(2)	39(2)	45(2)	4(1)	-7(1)	-6(1)
Cl(6)	40(2)	33(1)	38(2)	4(1)	-1(1)	0(1)
Sb(34)	22(1)	22(1)	21(1)	1(1)	2(1)	0(1)
Bi(2)	22(1)	22(1)	21(1)	1(1)	2(1)	0(1)
Cl(7)	63(2)	33(2)	30(2)	-4(1)	5(1)	2(1)
Cl(8)	51(2)	46(2)	52(2)	-2(2)	22(2)	-6(2)
Cl(9)	43(2)	34(1)	34(2)	1(1)	5(1)	0(1)
Cl(10)	38(2)	43(2)	36(2)	2(1)	2(1)	6(1)
Cl(11)	40(2)	42(2)	35(2)	0(1)	8(1)	-3(1)
Cl(12)	37(2)	44(2)	49(2)	-4(1)	2(1)	11(1)
Sb(35)	24(1)	23(1)	24(1)	-2(1)	3(1)	0(1)
Bi(1)	24(1)	23(1)	24(1)	-2(1)	3(1)	0(1)
O(36)	107(7)	57(5)	76(6)	35(5)	55(5)	21(4)
N(13)	33(4)	37(4)	34(4)	-1(3)	1(3)	-1(3)
N(14)	34(4)	40(4)	24(3)	1(3)	2(3)	4(3)
C(19)	34(5)	44(5)	43(5)	-4(4)	7(4)	-3(4)
C(20)	36(4)	34(4)	30(4)	0(4)	6(4)	2(3)
C(21)	34(4)	36(4)	32(4)	-4(4)	5(3)	-2(4)
C(22)	39(5)	38(5)	42(5)	-8(4)	-1(4)	-1(4)
C(23)	34(5)	47(5)	36(5)	8(4)	11(4)	7(4)
N(15)	36(4)	47(4)	40(4)	-3(3)	1(3)	-4(3)
N(16)	42(4)	35(4)	47(5)	2(3)	1(3)	3(3)
C(24)	54(6)	41(5)	34(5)	9(4)	7(4)	7(4)
C(25)	57(6)	30(4)	43(5)	3(4)	-7(4)	-1(4)
C(26)	49(5)	37(5)	34(5)	-5(4)	0(4)	-3(4)
C(27)	40(5)	41(5)	34(5)	-10(4)	3(4)	1(4)

C(28)	55(6)	48(6)	40(5)	-13(5)	11(4)	1(4)
N(17)	39(4)	40(4)	42(4)	-3(3)	5(3)	-4(3)
N(18)	41(4)	35(4)	38(4)	6(3)	7(3)	-1(3)
C(29)	38(5)	38(5)	46(5)	1(4)	1(4)	1(4)
C(30)	31(4)	39(5)	50(5)	1(4)	-3(4)	-2(4)
C(31)	39(5)	35(5)	41(5)	10(4)	1(4)	0(4)
C(32)	45(5)	47(5)	37(5)	1(4)	-1(4)	5(4)
C(33)	72(7)	38(5)	52(6)	0(5)	22(5)	-7(4)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S3.. Bond lengths [Å] for $(C_5H_{16}N_2)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}\cdot H_2O$ at 150.0 K with estimated standard deviations in parentheses.

Label	Distances	Label	Distances
Cl(1)-Bi(2)	2.636(2)	N(14)-C(21)	1.492(10)
Cl(2)-Bi(2)	2.683(2)	N(14)-C(22)	1.493(11)
Cl(3)-Bi(2)	2.709(2)	N(14)-C(23)	1.486(10)
Cl(4)-Bi(2)	2.802(2)	C(21)-C(20)	1.518(11)
Cl(5)-Bi(2)	2.735(2)	N(15)-C(27)	1.470(11)
Cl(6)-Bi(2)	2.673(2)	N(15)-C(28)	1.474(12)
Sb(34)-Cl(1)	2.636(2)	N(16)-C(24)	1.510(11)
Sb(34)-Cl(2)	2.683(2)	N(16)-C(25)	1.478(11)
Sb(34)-Cl(3)	2.709(2)	N(16)-C(26)	1.502(11)
Sb(34)-Cl(4)	2.802(2)	C(27)-C(26)	1.507(12)
Sb(34)-Cl(5)	2.735(2)	N(17)-C(31)	1.498(11)
Sb(34)-Cl(6)	2.673(2)	N(17)-C(32)	1.491(11)
Cl(8)-Sb(35)	2.652(2)	N(17)-C(33)	1.493(12)
Cl(9)-Sb(35)	2.573(2)	N(18)-C(29)	1.479(11)
Cl(10)-Sb(35)	2.718(2)	N(18)-C(30)	1.491(11)
Cl(11)-Sb(35)	2.712(2)	C(30)-C(31)	1.520(12)
Cl(12)-Sb(35)	2.637(2)	N(14)-C(21)	1.492(10)
Bi(1)-Cl(7)	2.913(2)	N(14)-C(22)	1.493(11)
Bi(1)-Cl(8)	2.652(2)	N(14)-C(23)	1.486(10)
Bi(1)-Cl(9)	2.573(2)	C(21)-C(20)	1.518(11)
Bi(1)-Cl(10)	2.718(2)	N(15)-C(27)	1.470(11)
Bi(1)-Cl(11)	2.712(2)	N(15)-C(28)	1.474(12)
Bi(1)-Cl(12)	2.637(2)	N(16)-C(24)	1.510(11)
N(13)-C(19)	1.489(11)	N(16)-C(25)	1.478(11)
N(13)-C(20)	1.483(10)	N(16)-C(26)	1.502(11)

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond angles [°] for $(C_5H_{16}N_2)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}\cdot H_2O$ at 150.0 K with estimated standard deviations in parentheses.

Label	Angles		
Cl(1)-Sb(34)-Cl(2)	90.82(7)	Cl(8)-Bi(1)-Cl(10)	89.39(7)
Cl(1)-Sb(34)-Cl(3)	92.83(7)	Cl(8)-Bi(1)-Cl(11)	177.26(7)
Cl(1)-Sb(34)-Cl(4)	173.85(7)	Cl(9)-Bi(1)-Cl(7)	172.92(7)
Cl(1)-Sb(34)-Cl(5)	98.47(7)	Cl(9)-Bi(1)-Cl(8)	90.24(7)
Cl(1)-Sb(34)-Cl(6)	88.87(7)	Cl(9)-Bi(1)-Cl(10)	83.88(7)
Cl(2)-Sb(34)-Cl(3)	92.66(7)	Cl(9)-Bi(1)-Cl(11)	91.54(7)
Cl(2)-Sb(34)-Cl(4)	85.43(6)	Cl(9)-Bi(1)-Cl(12)	89.15(7)
Cl(2)-Sb(34)-Cl(5)	170.58(7)	Cl(10)-Bi(1)-Cl(7)	99.03(7)
Cl(3)-Sb(34)-Cl(4)	82.50(6)	Cl(11)-Bi(1)-Cl(7)	94.75(6)
Cl(3)-Sb(34)-Cl(5)	88.50(7)	Cl(11)-Bi(1)-Cl(10)	92.86(7)
Cl(5)-Sb(34)-Cl(4)	85.46(7)	Cl(12)-Bi(1)-Cl(7)	87.76(7)
Cl(6)-Sb(34)-Cl(2)	88.81(7)	Cl(12)-Bi(1)-Cl(8)	89.46(8)
Cl(6)-Sb(34)-Cl(3)	177.73(7)	Cl(12)-Bi(1)-Cl(10)	172.94(7)
Cl(6)-Sb(34)-Cl(4)	95.90(6)	Cl(12)-Bi(1)-Cl(11)	88.50(7)
Cl(6)-Sb(34)-Cl(5)	89.76(6)	C(20)-N(13)-C(19)	110.6(6)
Cl(1)-Bi(2)-Cl(2)	90.82(7)	C(21)-N(14)-C(22)	112.9(6)
Cl(1)-Bi(2)-Cl(3)	92.83(7)	C(23)-N(14)-C(21)	110.5(7)
Cl(1)-Bi(2)-Cl(4)	173.85(7)	C(23)-N(14)-C(22)	109.8(7)
Cl(1)-Bi(2)-Cl(5)	98.47(7)	N(13)-C(20)-C(21)	110.1(7)
Cl(1)-Bi(2)-Cl(6)	88.87(7)	N(14)-C(21)-C(20)	110.2(7)
Cl(2)-Bi(2)-Cl(3)	92.66(7)	C(27)-N(15)-C(28)	114.0(7)
Cl(2)-Bi(2)-Cl(4)	85.43(6)	C(25)-N(16)-C(24)	110.2(7)
Cl(2)-Bi(2)-Cl(5)	170.58(7)	C(25)-N(16)-C(26)	112.7(7)
Cl(3)-Bi(2)-Cl(4)	82.50(6)	C(26)-N(16)-C(24)	108.7(7)
Cl(3)-Bi(2)-Cl(5)	88.50(7)	N(16)-C(26)-C(27)	113.2(7)
Cl(5)-Bi(2)-Cl(4)	85.46(7)	N(15)-C(27)-C(26)	109.3(7)
Cl(6)-Bi(2)-Cl(2)	88.81(7)	C(32)-N(17)-C(31)	112.3(7)
Cl(6)-Bi(2)-Cl(3)	177.73(7)	C(32)-N(17)-C(33)	110.7(7)
Cl(6)-Bi(2)-Cl(4)	95.90(6)	C(33)-N(17)-C(31)	109.6(7)
Cl(6)-Bi(2)-Cl(5)	89.76(6)	C(29)-N(18)-C(30)	115.4(7)
Cl(8)-Sb(35)-Cl(10)	89.39(7)	N(18)-C(30)-C(31)	109.5(7)
Cl(8)-Sb(35)-Cl(11)	177.26(7)	N(17)-C(31)-C(30)	111.4(7)
Cl(9)-Sb(35)-Cl(8)	90.24(7)	Cl(12)-Sb(35)-Cl(10)	172.94(7)
Cl(9)-Sb(35)-Cl(10)	83.88(7)	Cl(12)-Sb(35)-Cl(11)	88.50(7)

Cl(9)-Sb(35)-Cl(11)	91.54(7)	Cl(8)-Bi(1)-Cl(7)	83.36(7)
Cl(9)-Sb(35)-Cl(12)	89.15(7)	Cl(8)-Bi(1)-Cl(10)	89.39(7)
Cl(11)-Sb(35)-Cl(10)	92.86(7)	Cl(8)-Bi(1)-Cl(11)	177.26(7)
Cl(12)-Sb(35)-Cl(8)	89.46(8)	Cl(9)-Bi(1)-Cl(7)	172.92(7)
Cl(12)-Sb(35)-Cl(10)	172.94(7)	Cl(9)-Bi(1)-Cl(8)	90.24(7)
Cl(12)-Sb(35)-Cl(11)	88.50(7)	Cl(9)-Bi(1)-Cl(10)	83.88(7)
Cl(8)-Bi(1)-Cl(7)	83.36(7)	Cl(9)-Bi(1)-Cl(11)	91.54(7)

Symmetry transformations used to generate equivalent atoms:

Table S5. (The lead content for the metal components in the raw material and that obtained from EDS experiment)

Raw Material (Sb%)	0.1	0.2	0.3	0.4	0.5	0.6
Experiment (Sb%)	0.06	0.12	0.17	0.24	0.32	0.44

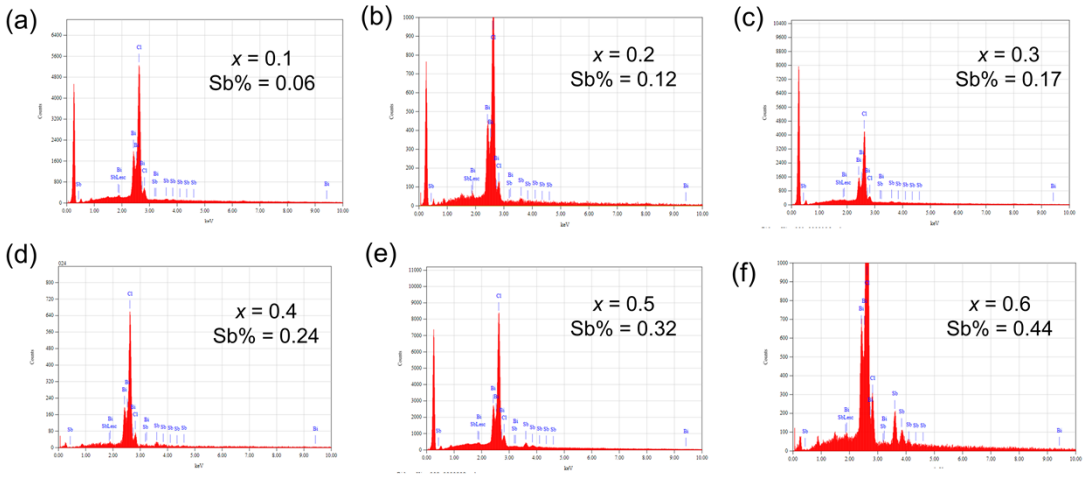

Figure S1. The EDS analysis of content of Sb for metal components in $(TMEDA)_3(Sb_xBi_{1-x})_2Cl_{12}\cdot H_2O$ (x = 0.1-0.6).

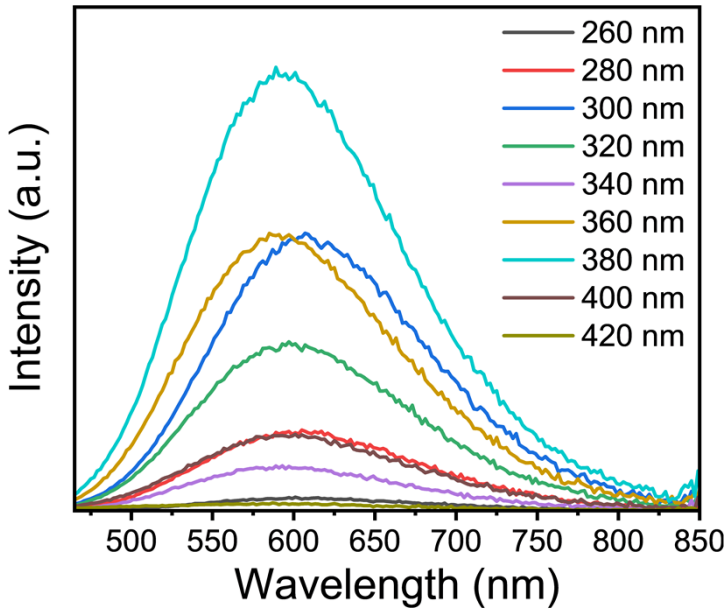

Figure S2. PL spectra of $(TMEDA)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}\cdot H_2O$ upon excitation at different wavelengths at RT.

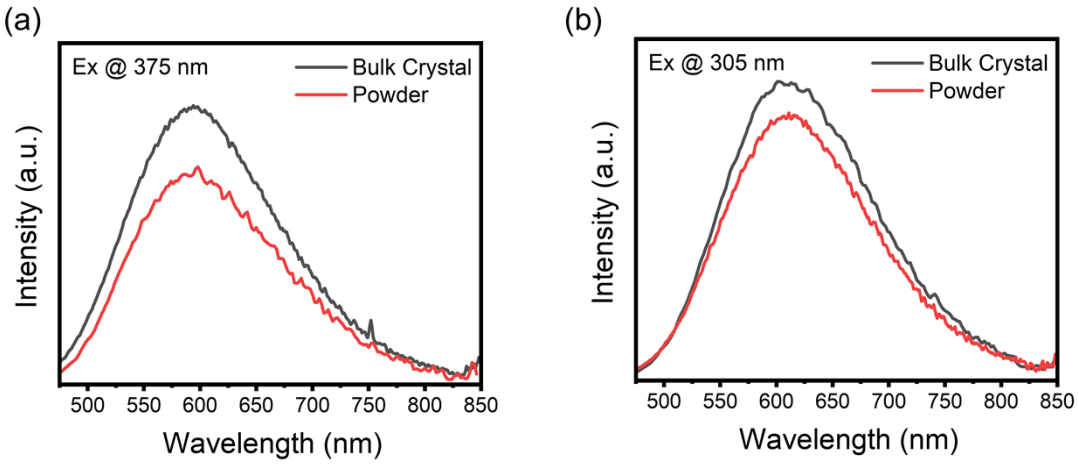

Figure S3. Comparison of emission spectra for bulk crystal and powder of $(TMEDA)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}\cdot H_2O$

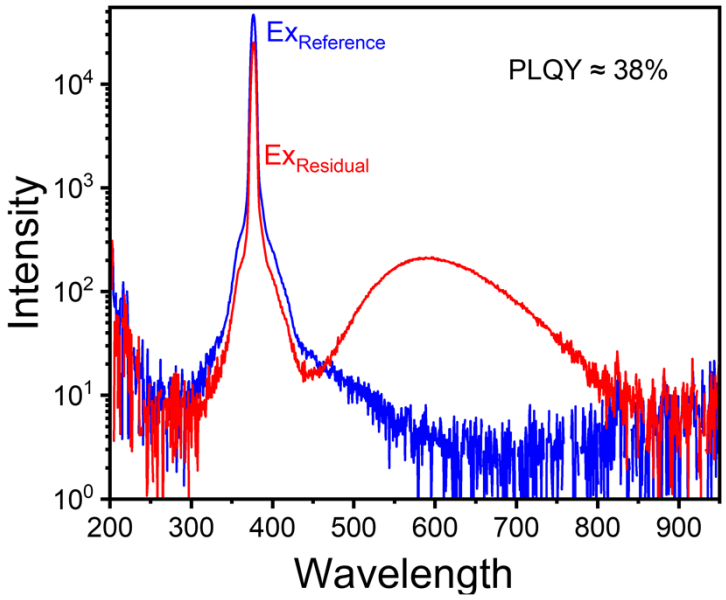

Figure S4. PLQYs spectra of $(TMEDA)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}\cdot H_2O$

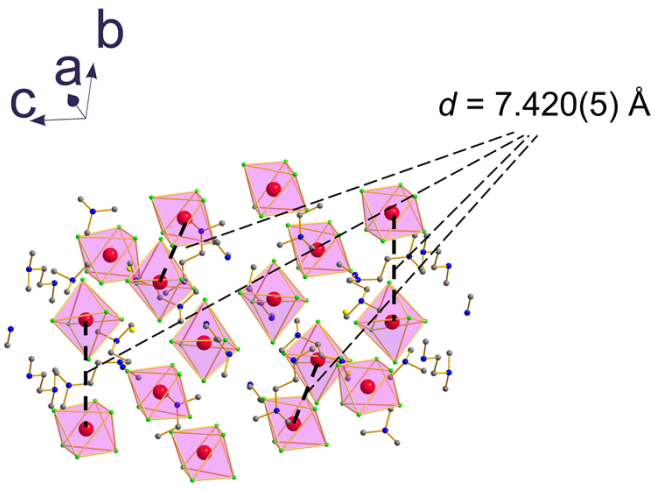

Figure S5. The M···M distances: 7.4197(5) Å (shortest) in crystal structure of $(TMEDA)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}\cdot H_2O$, labeled with black thick dashed line.

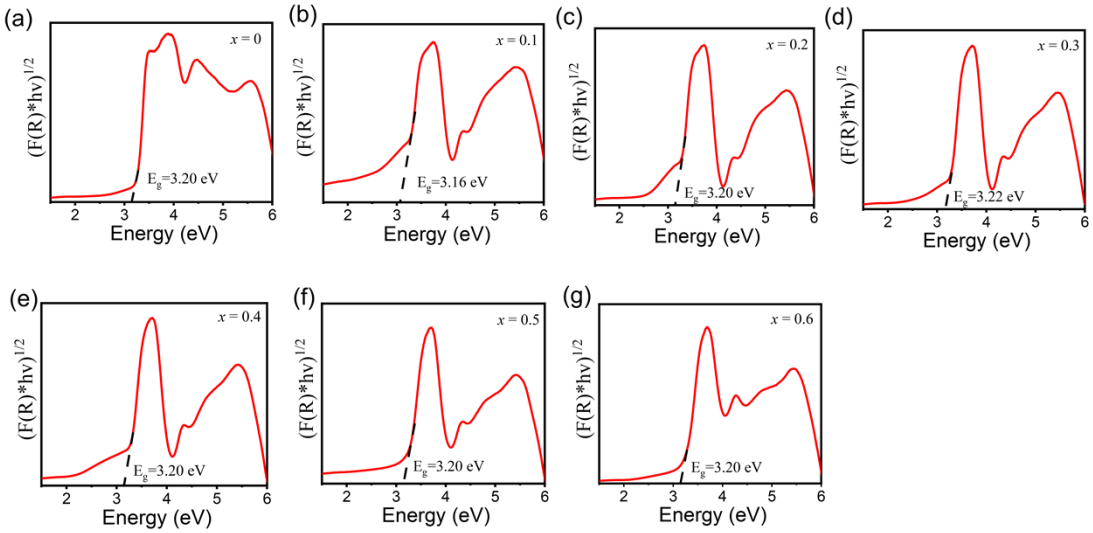

Figure S6. the band gap of $TMEDA)_3(Sb_xBi_{1-x})_2Cl_{12}\cdot H_2O$ (x = 0-0.6) determined from a Tauc plot**.**

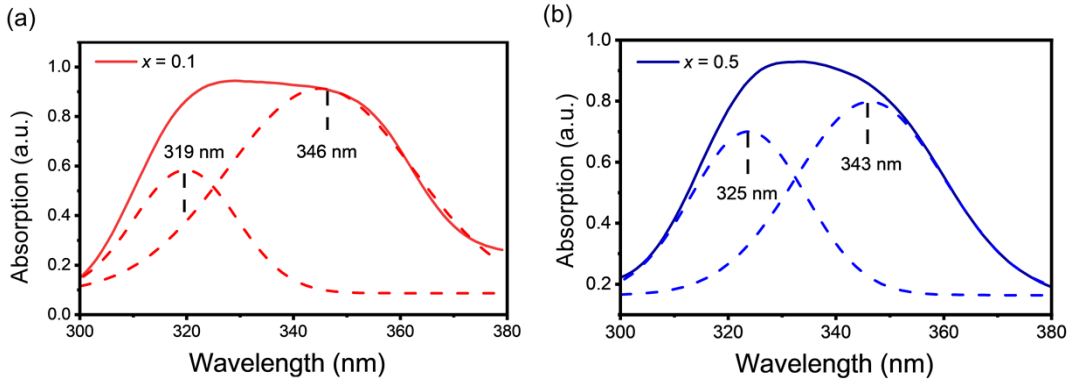

Figure S7. Split fitting of absorption peaks (300-380 nm) for x = 0.1 and x = 0.5.

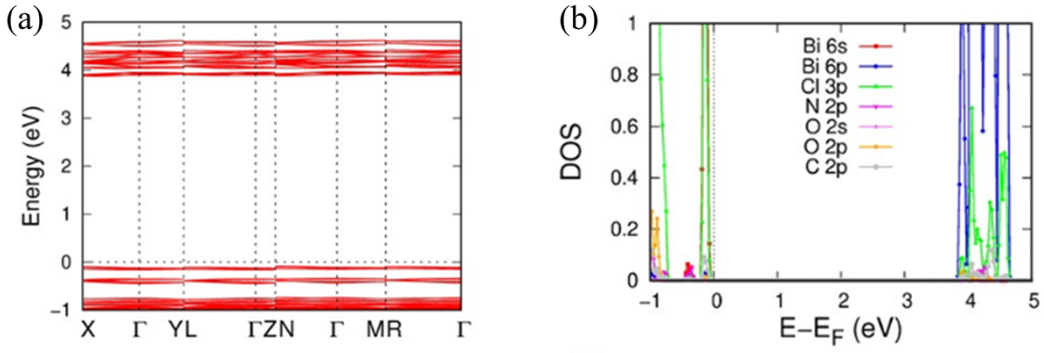

Figure S8 Band structures of $(TMEDA)_3Bi_2Cl_{12}\cdot H_2O$ (a), DOS of $(TMEDA)_3Bi_2Cl_{12}\cdot H_2O$ (b).

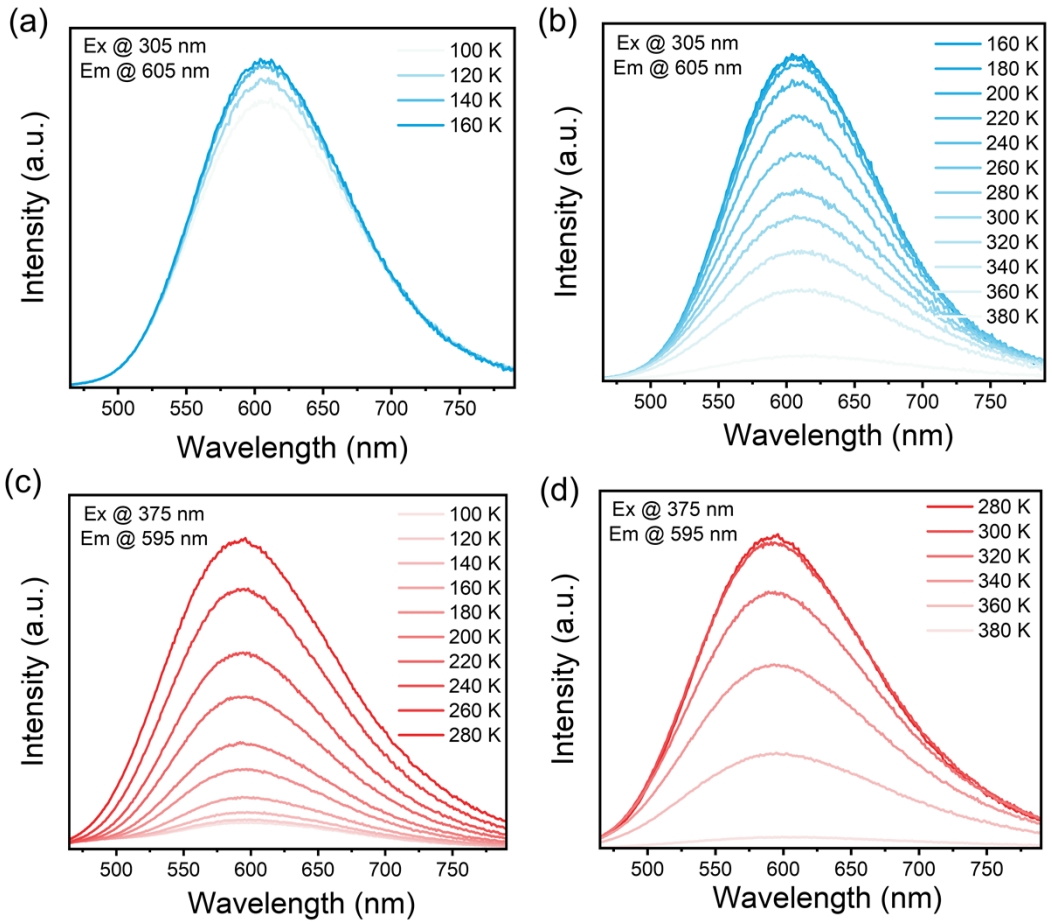

Figure S9. Temperature-dependent PL spectra of $(TMEDA)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}\cdot H_2O$, for the emission at 605 nm (Ex = 305 nm), 100–160 K (a), 160–380 K (b); for the emission at 595 nm (Ex = 375 nm), 100–280 K (a), 280–380 K (b).

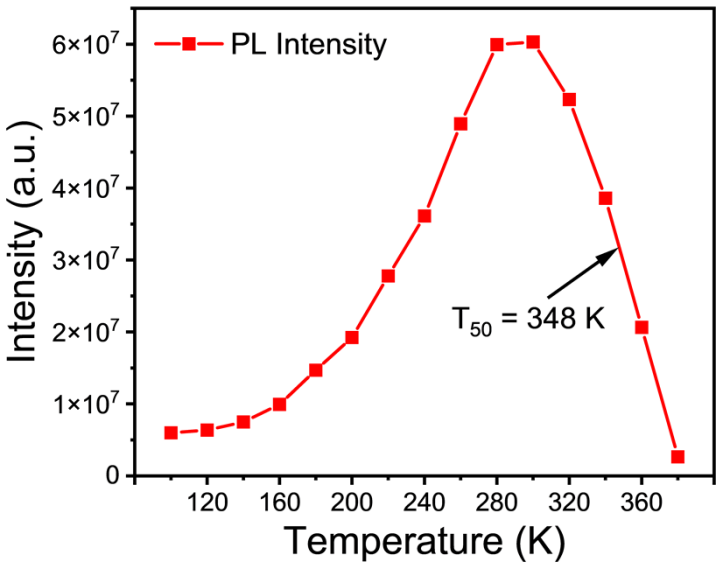

Figure S10. The PL integrated intensity variation spectrum of

$(TMEDA)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}·H_2O$ in the range of 100 -380 K (Ex = 375 nm, Em = 595 nm).

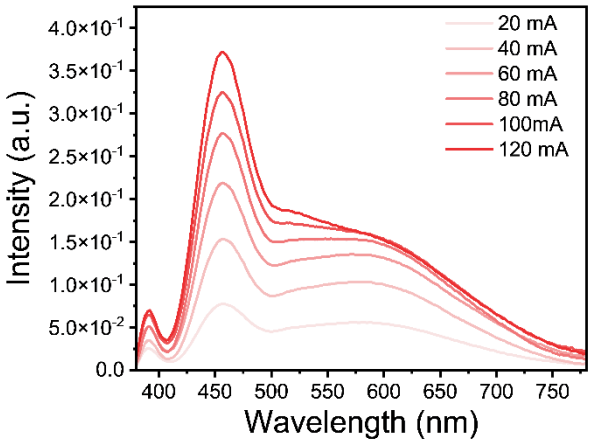

Figure S11. Electroluminescence spectrum of $(TMEDA)_3(Sb_{0.5}Bi_{0.5})_2Cl_{12}·H_2O$ – based WLED.