

Supporting Information

Boosting the broadband orange emission in organic-inorganic hybrid metal halide of (DPG)₃InBr₆ via antimony doping

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Table S1 Crystal data and structure refinement for (DPG)₃InBr₆.

Empirical formula	(DPG) ₃ InBr ₆
Chemical formula	C ₃₉ H ₄₂ Br ₆ InN ₉
Formula weight	1231.05
Temperature (K)	296.15
Crystal system	Trigonal
Space group	R-3
a (Å)	<i>a</i> = 16.613(3)Å
b (Å)	<i>b</i> = 16.613Å
c (Å)	<i>c</i> = 14.280(3)Å
α (deg)	α = 90°
β (deg)	β = 90°
γ (deg)	γ = 120°
Volume (Å ³)	3413.1(13)
Z	3
Density (calculated) (g·cm ⁻³)	1.797
Absorption coefficient (mm ⁻¹)	5.826
<i>F</i> (000)	1794
Index ranges	-21 ≤ <i>h</i> ≤ 15, -17 ≤ <i>k</i> ≤ 20, -18 ≤ <i>l</i> ≤ 14
Reflections collected	88712
Data completeness	99.9%
Data/restraints/parameters Goodness-of-fit	1740/0/132
Goodness of fit	1.013
R (reflections)	0.0288
wR2 (reflections)	0.0750
Largest diff. peak and hole (eÅ ⁻³)	0.7 and -0.5

Table S2 Bond angles of (DPG)₃InBr₆ and (DPG)₃InBr₆: Sb single crystal.

(DPG) ₃ InBr ₆	Geometry	Br1-In1-Br2	Br1-In1-Br3	Br1-In1-Br4
	Bond angle	88.1365°	88.1412°	91.8683°
	Geometry	Br1-In1-Br5	Br2-In1-Br3	Br3-In1-Br4
	Bond angle	91.8633°	91.8623°	88.141°
	Geometry	Br4-In1-Br5	Br5-In1-Br2	Br2-In1-Br1
	Bond angle	91.8628°	88.1340°	91.8595°
	Geometry	Br3-In1-Br1	Br4-In1-Br1	Br5-In1-Br1
	Bond angle	91.8620°	88.1357°	88.1334°
(DPG) ₃ InBr ₆ : Sb	Geometry	Br1-In1-Br5	Br3-In1-Br5	Br1-In1-Br4
	Bond angle	83.6459°	91.3516°	91.8897°
	Geometry	Br3-In1-Br4	Br4-In1-Br5	Br2-In1-Br5
	Bond angle	88.6608°	87.0720°	91.0878°
	Geometry	Br3-In1-Br6	Br1-In1-Br6	Br2-In1-Br3
	Bond angle	91.7631°	93.2307°	93.1254°
	Geometry	Br2-In1-Br1	Br2-In1-Br6	Br4-In1-Br6
	Bond angle	86.1734°	88.1281°	93.6156°

Table S3 Bond lengths of (DPG)₃InBr₆ and (DPG)₃InBr₆: Sb single crystal.

(DPG) ₃ InBr ₆	Geometry	In1-Br1	In1-Br3	In1-Br5
	Bond length	2.67738 Å	2.67758 Å	2.67763 Å
	Geometry	In1-Br2	In1-Br4	In1-Br6
	Bond length	2.6774 Å	2.67747 Å	2.67759 Å
(DPG) ₃ InBr ₆ : Sb	Geometry	In1-Br1	In1-Br3	In1-Br5

	Bond length	2.70673 Å	2.70649 Å	2.71687 Å
	Geometry	In1-Br2	In1-Br4	In1-Br6
	Bond length	2.74784 Å	2.716840 Å	2.73621 Å

Table S4 Time-resolved PL decay curve of $(\text{DPG})_3\text{InBr}_6$ with different doping concentrations (EX: 405 nm laser, EM: 630 nm).

	$(\text{DPG})_3\text{InBr}_6$	$(\text{DPG})_3\text{InBr}_6$: 1%Sb	$(\text{DPG})_3\text{InBr}_6$: 5%Sb	$(\text{DPG})_3\text{InBr}_6$: 10%Sb	$(\text{DPG})_3\text{InBr}_6$: 30%Sb
τ_1	4.3 ns (70.8%)	9.3 ns (65.3%)	11.1 ns (32.9%)	-	-
τ_2	2.0 μs (29.2%)	1.9 μs (34.7%)	1.7 μs (67.1%)	1.6 μs	1.6 μs

Table S5 Time-resolved PL decay curve of $(\text{DPG})_3\text{InBr}_6$ with different doping concentrations (EX: 405 nm laser, EM: 470 nm).

	$(\text{DPG})_3\text{InBr}_6$	$(\text{DPG})_3\text{InBr}_6$: 1%Sb	$(\text{DPG})_3\text{InBr}_6$: 5%Sb	$(\text{DPG})_3\text{InBr}_6$: 10%Sb	$(\text{DPG})_3\text{InBr}_6$: 30%Sb
τ_1	1.9 ns	1.9 ns	2.6 ns	1.4 ns	1.6 ns

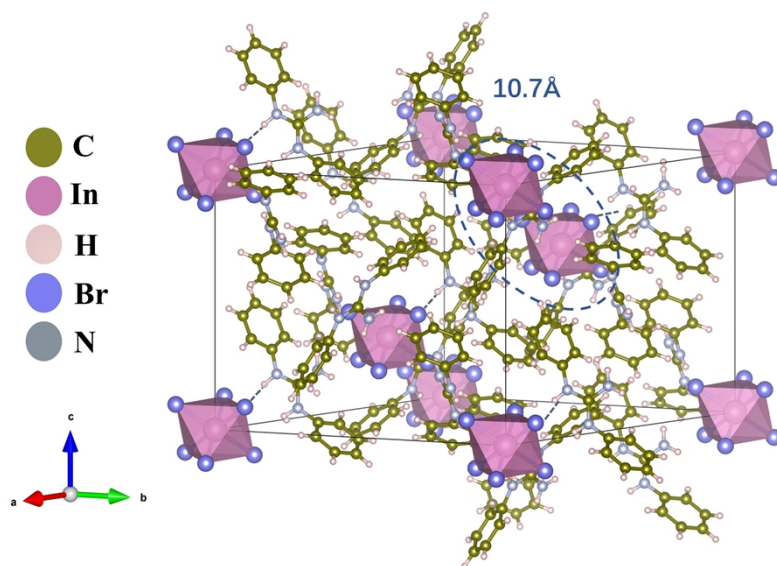


Fig. S1 Crystal structure of $(\text{DPG})_3\text{InBr}_6$.

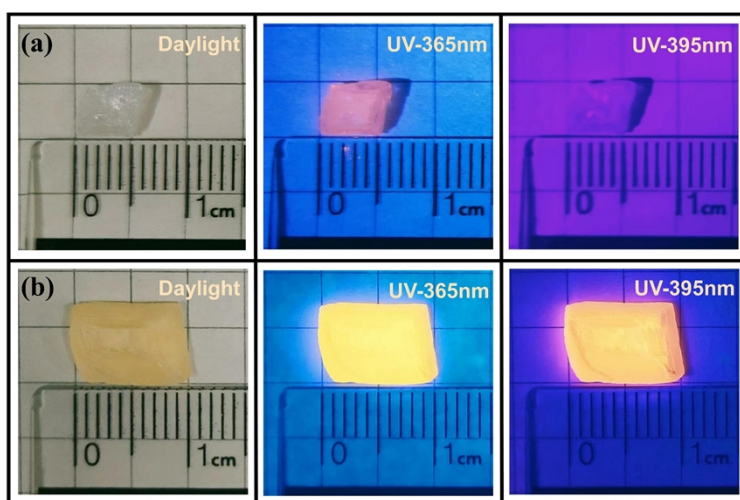


Fig. S2 Images of $(\text{DPG})_3\text{InBr}_6$ (a) and $(\text{DPG})_3\text{InBr}_6$: 10% Sb. (b) single crystals under daylight and UV-365 nm & 395 nm excitation.

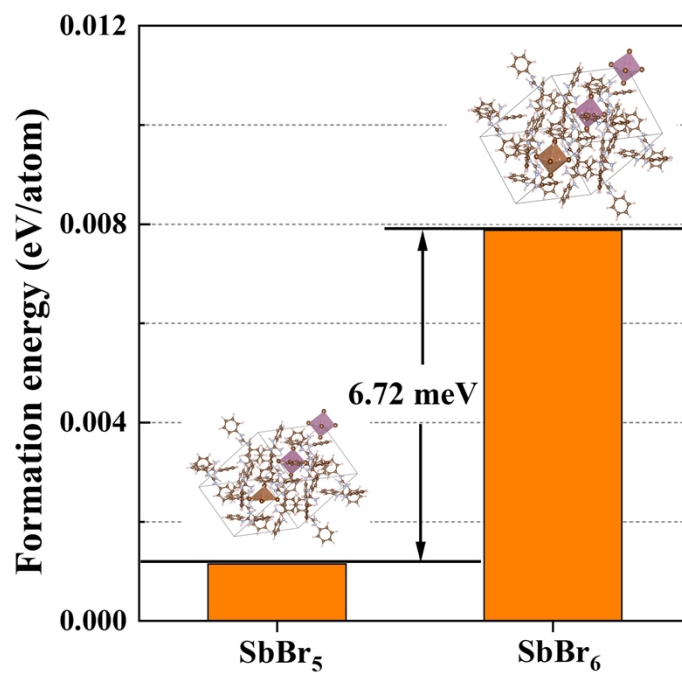


Fig. S3 Formation energy for $(\text{DPG})_3\text{InBr}_6$: Sb with five and six coordination numbers.

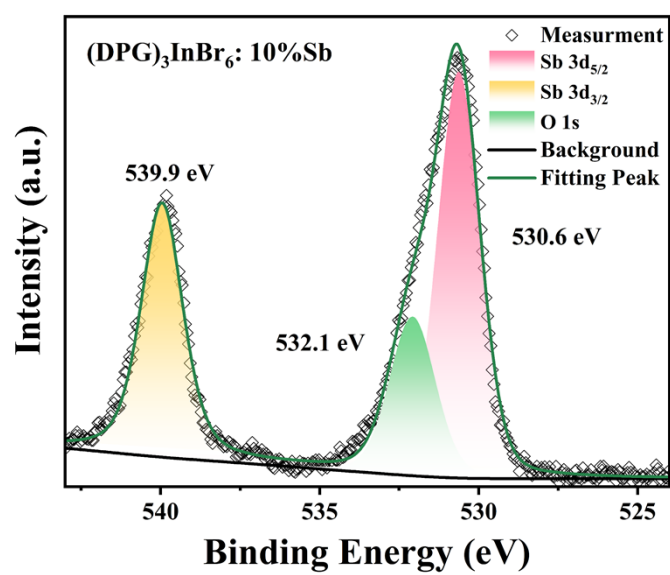


Fig. S4 High-resolution XPS spectra of O 1s and Sb $3d_{3/2}$ and $3d_{5/2}$ for $(\text{DPG})_3\text{InBr}_6$: 10% Sb.

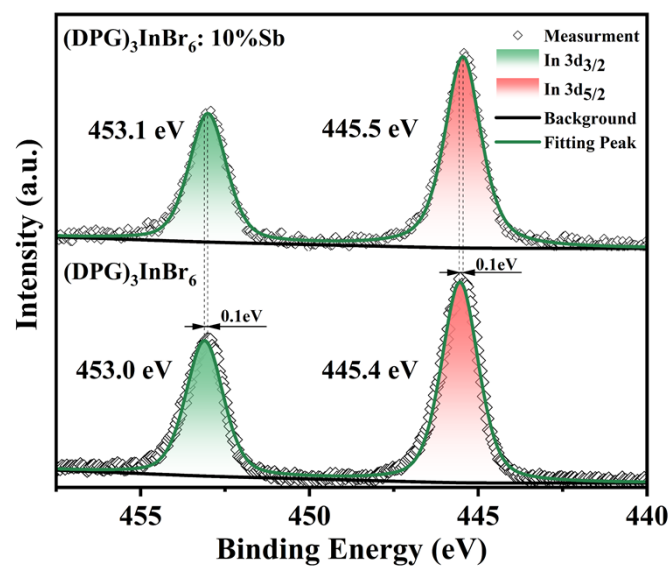


Fig. S5 High-resolution XPS image of $(\text{DPG})_3\text{InBr}_6$ and $(\text{DPG})_3\text{InBr}_6: 10\% \text{Sb}$.

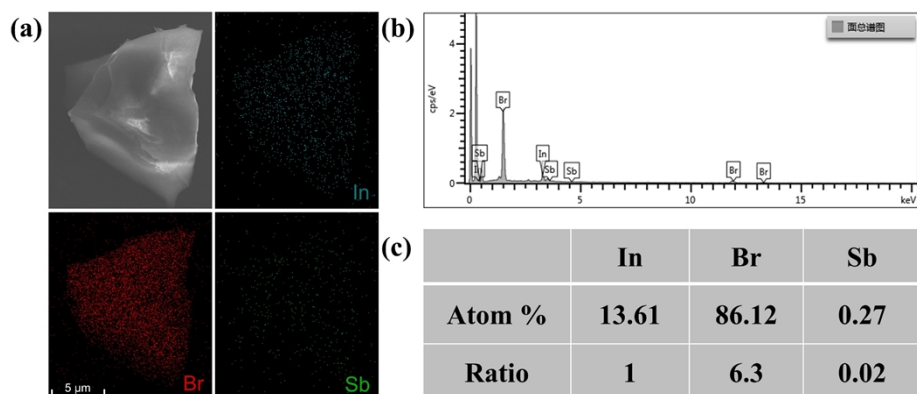


Fig. S6 (a) SEM image and the corresponding EDS mapping of elements. (b) EDS spectrum and (c) atomic percent of elements in the $(\text{DPG})_3\text{InBr}_6: 5\% \text{Sb}$. Scale bar: 5 μm .

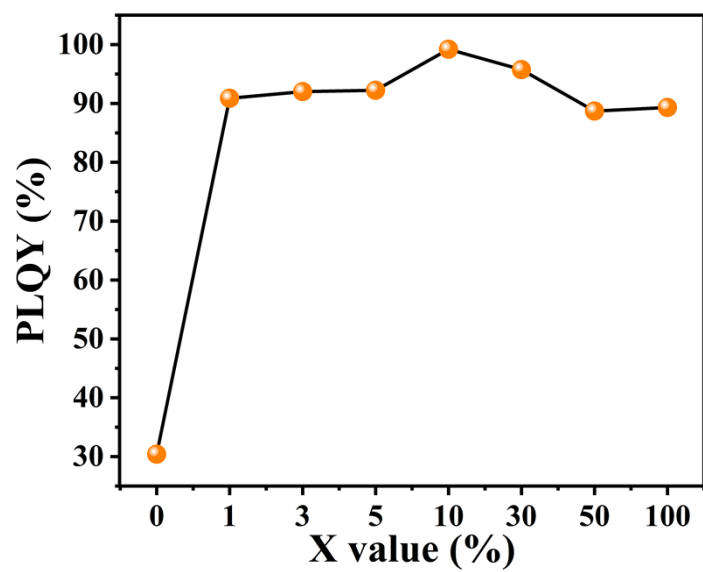


Fig. S7 The PLQY of $(\text{DPG})_3\text{InBr}_6: x\%\text{Sb}$ ($x=0, 1, 3, 5, 10, 30, 50, 100$).

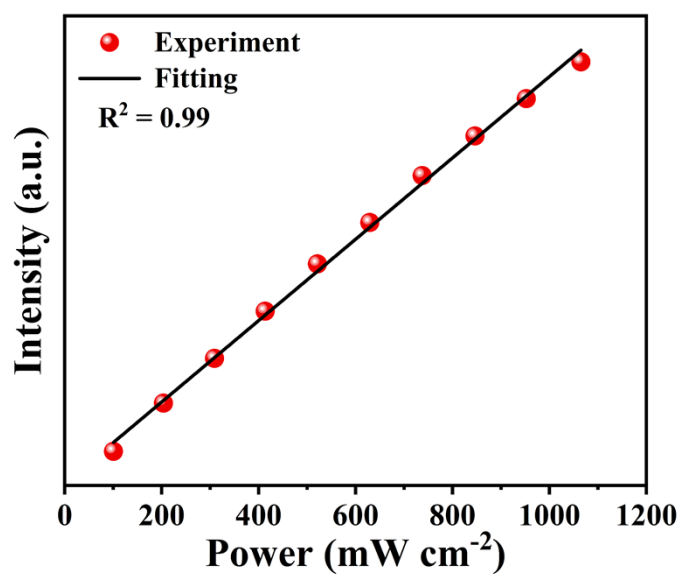


Fig. S8 PL intensity versus excitation power for $(\text{DPG})_3\text{InBr}_6: 10\%\text{Sb}$.

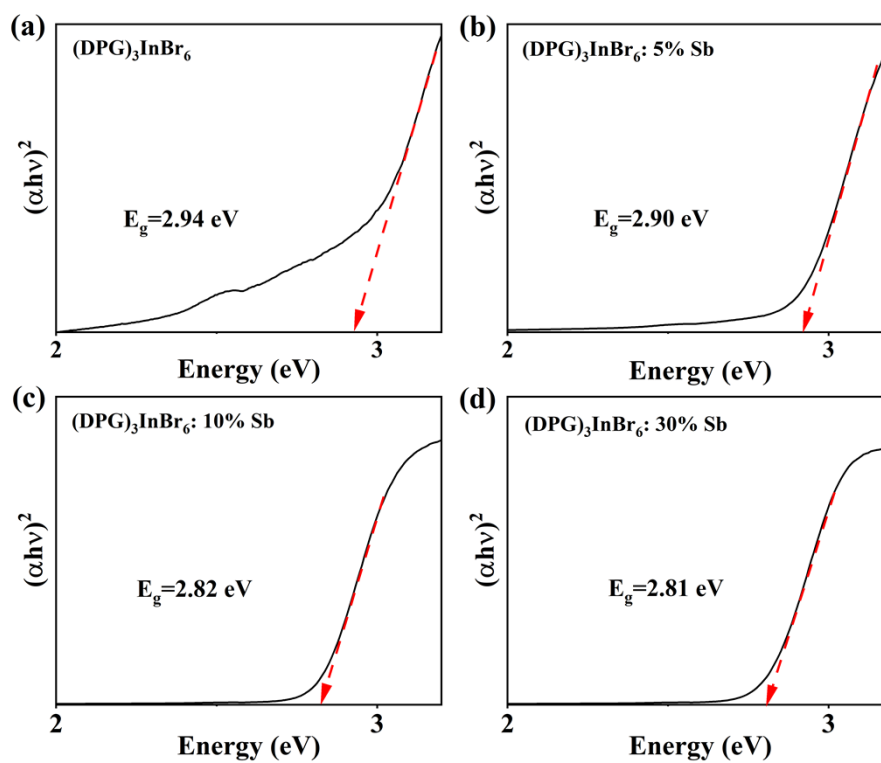


Fig. S9 The Tauc plots of $(\text{DPG})_3\text{InBr}_6$ with different Sb doping concentrations.

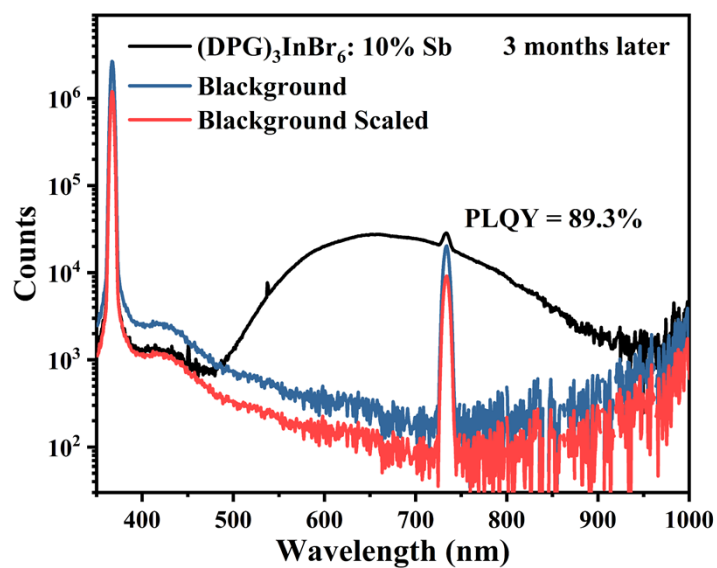


Fig. S10 PLQY measurement of $(\text{DPG})_3\text{InBr}_6$: 10% Sb after 3 months.

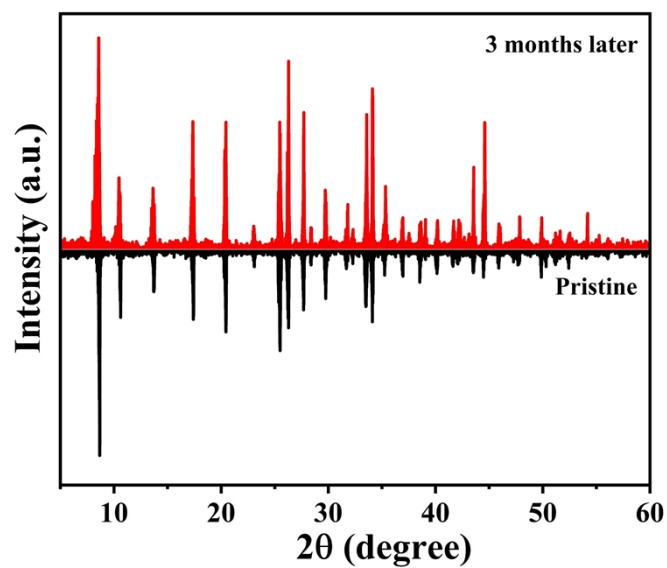


Fig. S11 PXR D patterns of (DPG)₃InBr₆: 10% Sb before and after 3 months.

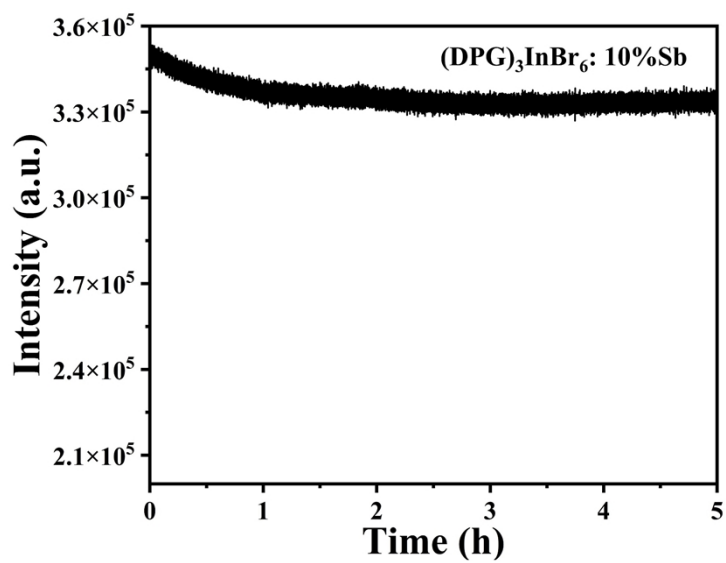


Fig. S12 Photostability of (DPG)₃InBr₆: 10% Sb under continuous excitation (380 nm, 150mW cm⁻²).

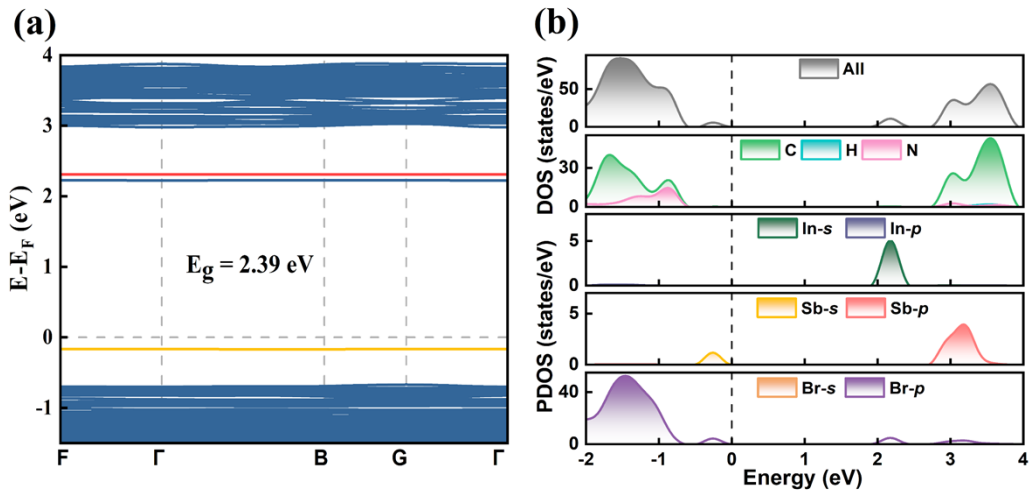


Fig. S13 the DFT calculations of electronic band structure and DOS of $(DPG)_3InBr_6$: Sb with six coordination.

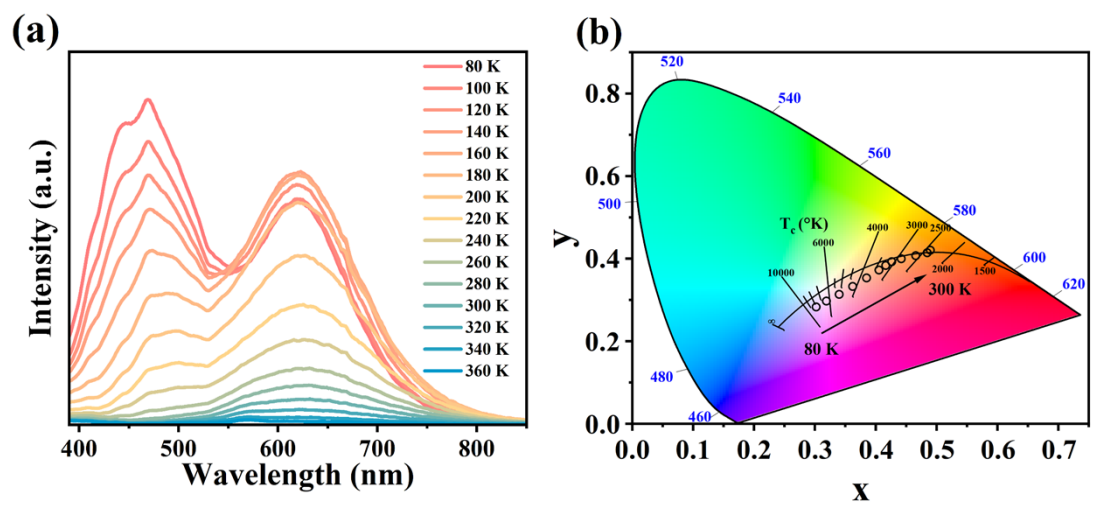


Fig. S14 (a) Emission spectrum of $(DPG)_3InBr_6$ at different temperatures excited at 322nm. (b) CIE coordinates of $(DPG)_3InBr_6$ at different temperatures.

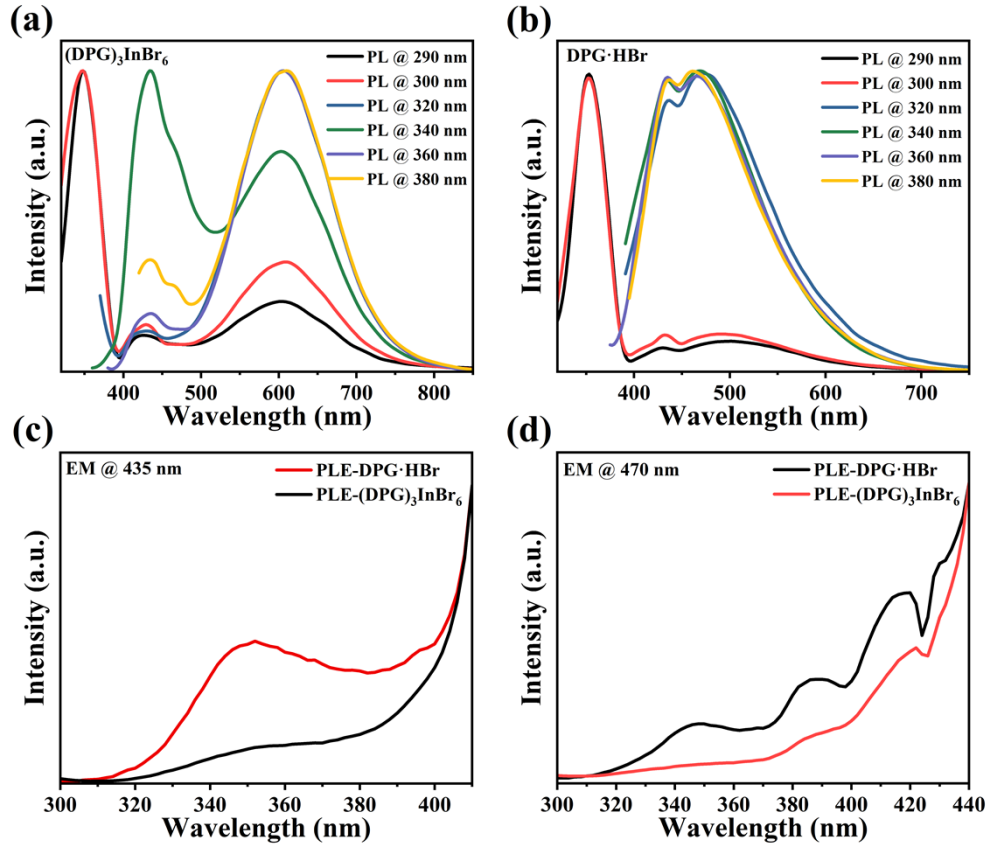


Fig. S15 (a) The excitation-wavelength dependent PL spectra of $(\text{DPG})_3\text{InBr}_6$ (b) and $\text{DPG}\cdot\text{HBr}$. (c) PLE spectra of $(\text{DPG})_3\text{InBr}_6$ and $\text{DPG}\cdot\text{HBr}$ monitored at 435 (d) and 470 nm.

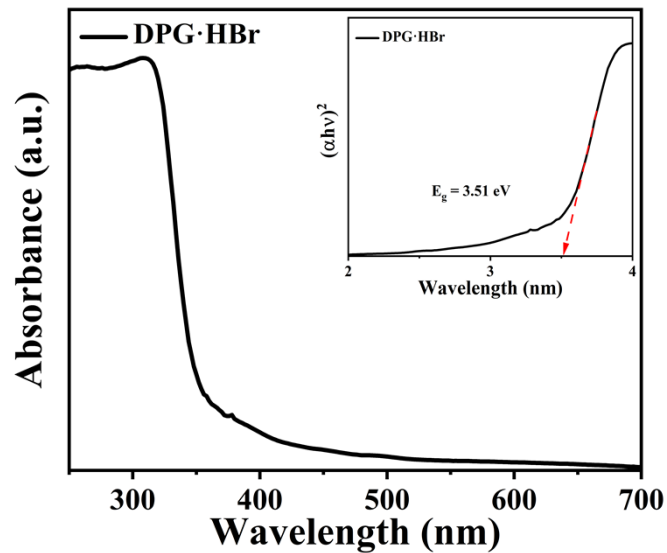


Fig. S16 Absorption spectra of $\text{DPG}\cdot\text{HBr}$, Insert: Tauc plot of $\text{DPG}\cdot\text{HBr}$.

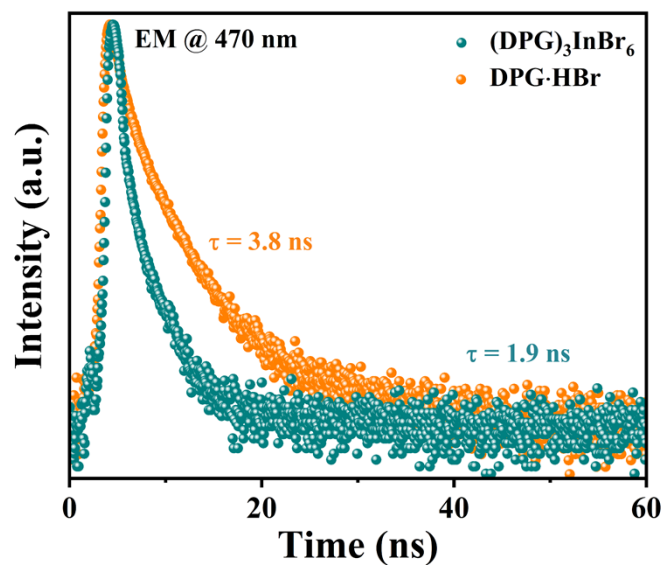


Fig. S17 Time-resolved PL decay curve of $(\text{DPG})_3\text{InBr}_6$ and $\text{DPG}\cdot\text{HBr}$ monitored at 470 nm.

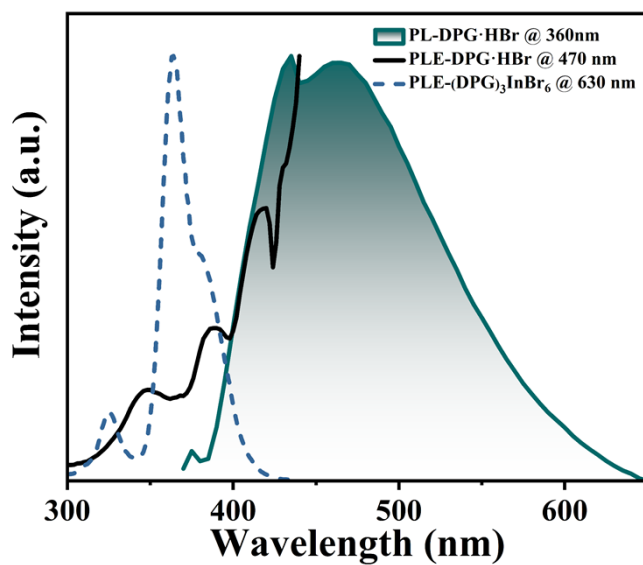


Fig. S18 PL of $\text{DPG}\cdot\text{HBr}$ monitored at 360 nm and PLE spectra of $\text{DPG}\cdot\text{HBr}$ monitored at 470 nm and $(\text{DPG})_3\text{InBr}_6$ monitored at 630 nm.