

Supporting Information

Dual Blue Fluorescence and Green Phosphorescence of Hybrid Cadmium Halide for Anti-counterfeiting

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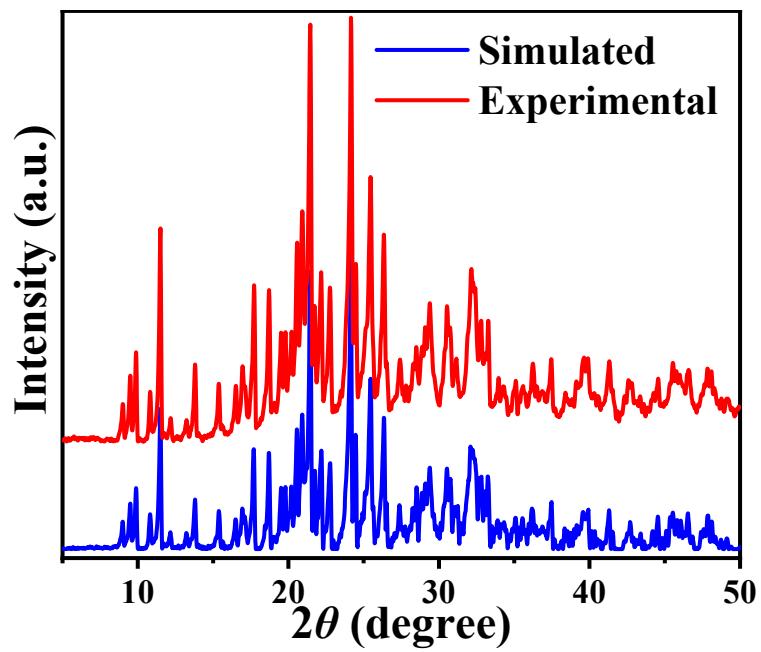


Fig. S1. Experimental and simulated PXRD patterns of [BTPP]Br.

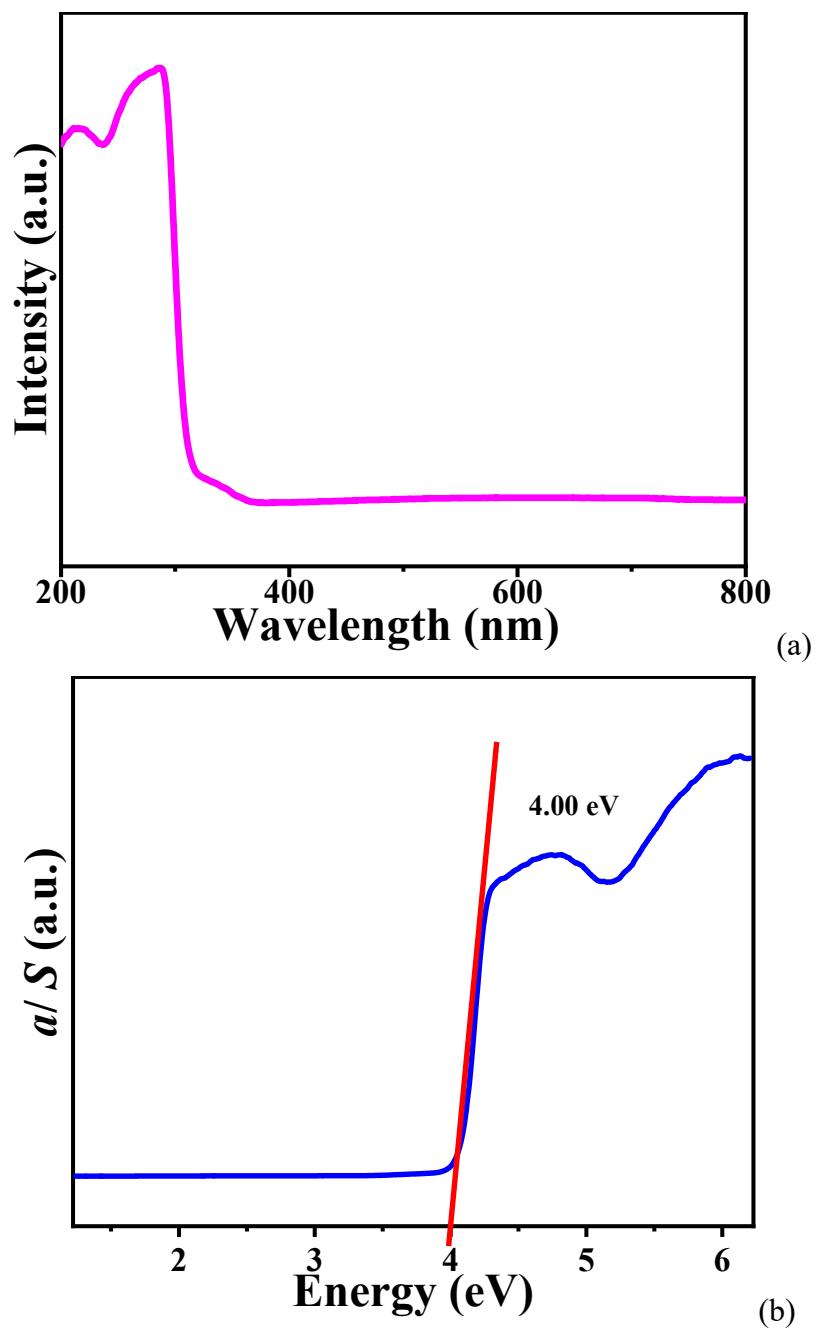


Fig. S2. The solid-state UV-Vis absorption spectra *vs* wavelength (a) and photo energy (b) of $[\text{BTPP}]\text{Br}$ at 300 K.

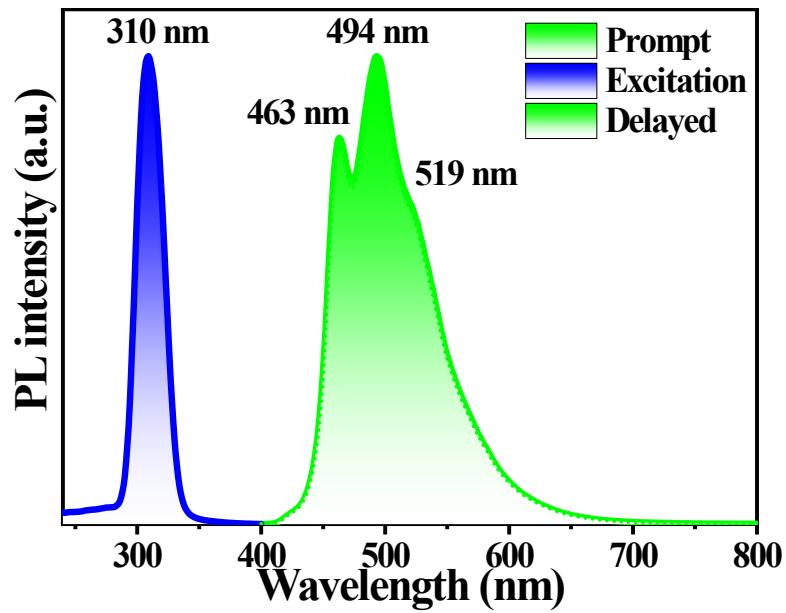
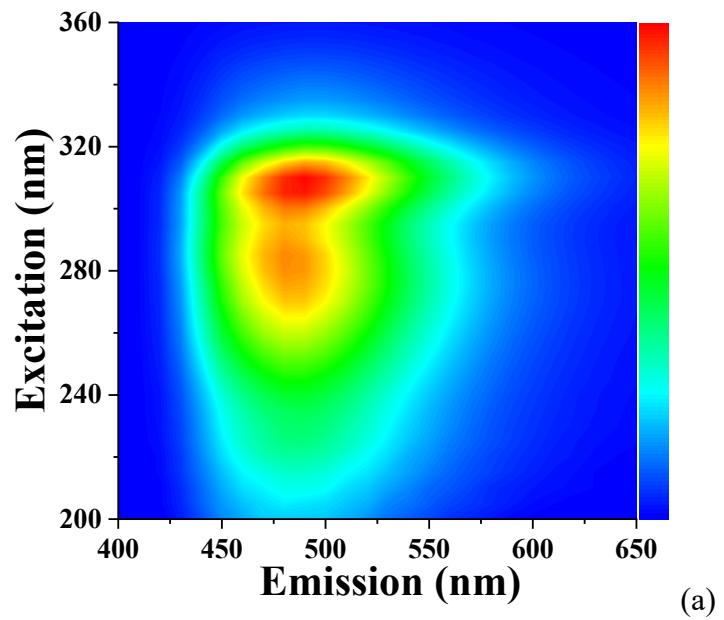
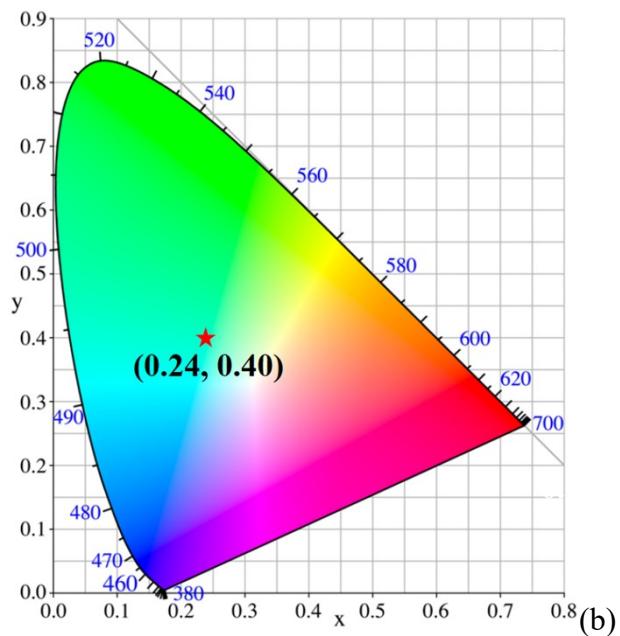


Fig. S3. The PL excitation and emission spectra of [BTPP]Br in prompt- and delayed-mode.



(a)



(b)

Fig. S4. 3D consecutive PL excitation-emission correlation map (a) and the corresponding CIE coordinates (b) of [BTPP]Br at 300 K.

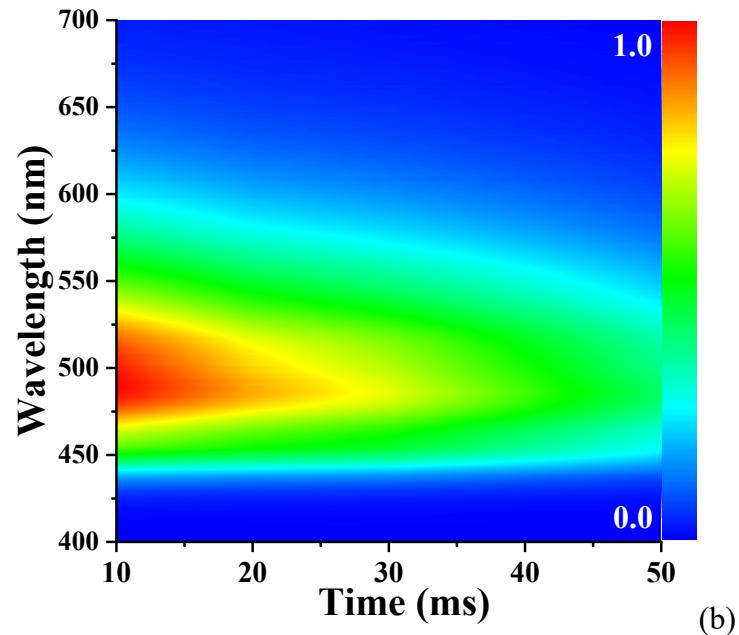
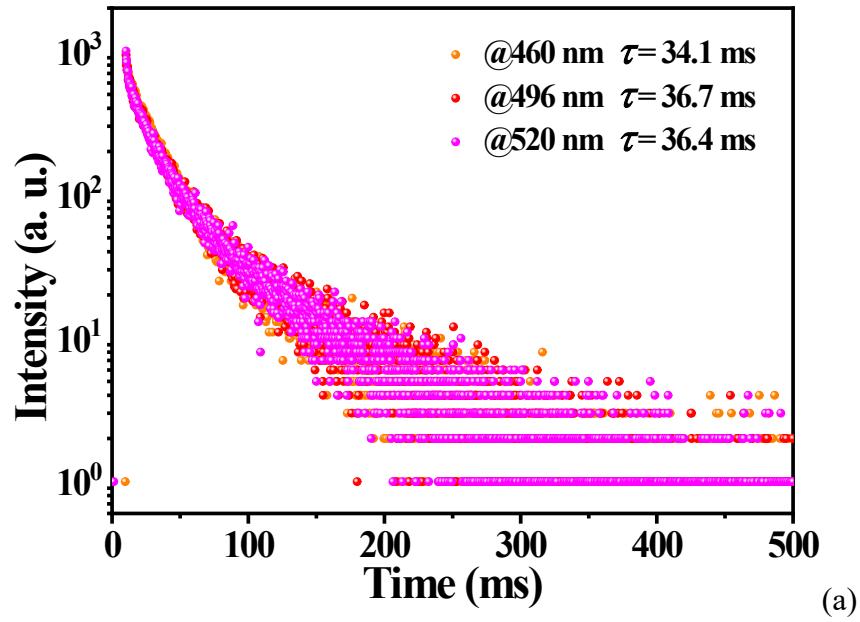


Fig. S5. The PL decay curves monitoring at 463 nm, 494 nm and 519 nm excited by 310 nm (a), Time-resolved transient emission spectra (b) of [BTPP]Br at 300 K.

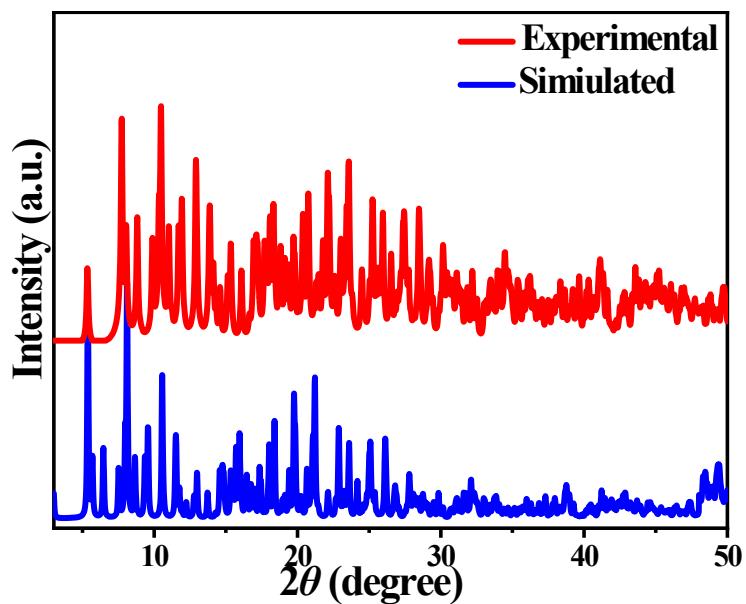


Fig. S6. Experimental and simulated PXRD patterns of $[BTPP]_2CdBr_4$.

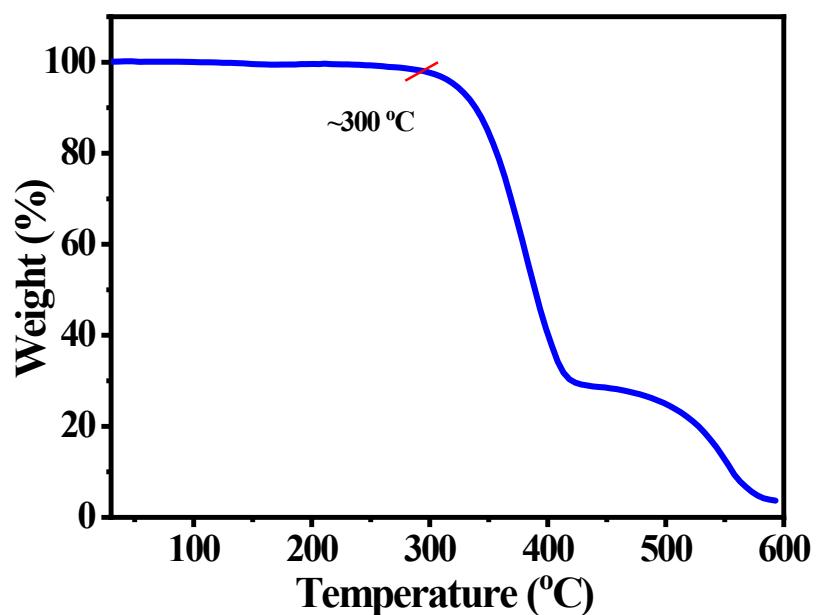


Fig. S7. The thermogravimetric analysis curve of $[BTPP]_2CdBr_4$.

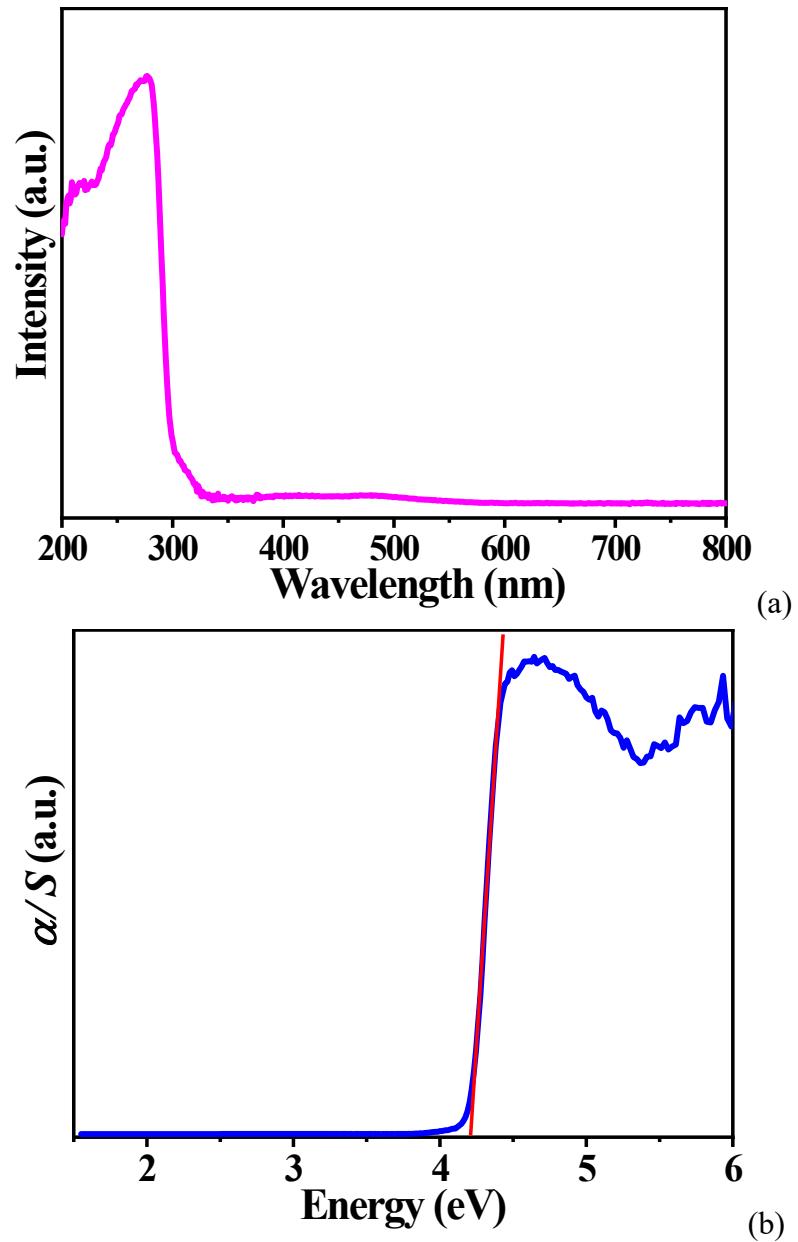


Fig. S8. The solid-state UV-Vis absorption spectra *vs* wavelength (a) and photo energy (b) of $[\text{BTPP}]_2\text{CdBr}_4$ at 300 K.

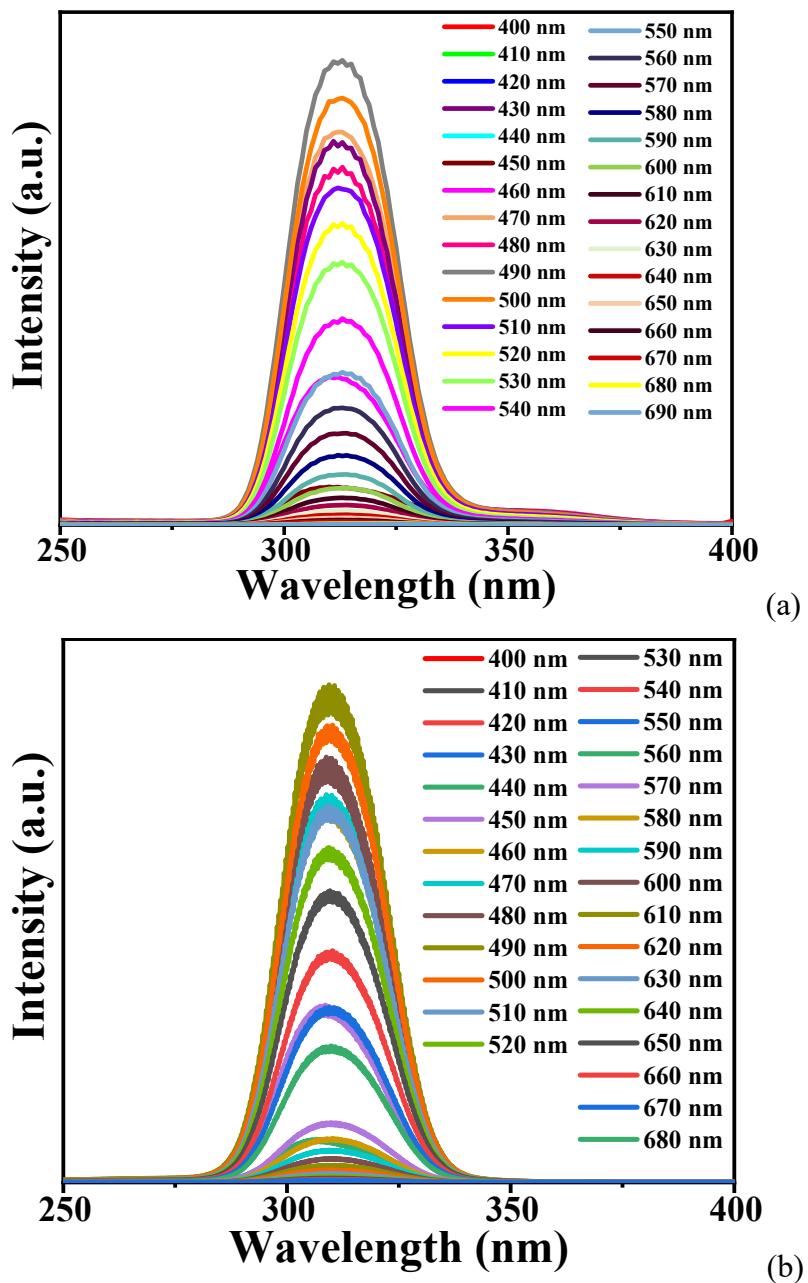


Fig. S9. The prompt-mode (a) and delayed-mode (b) emission wavelength dependent PL excitation spectra of $[BTPP]_2CdBr_4$.

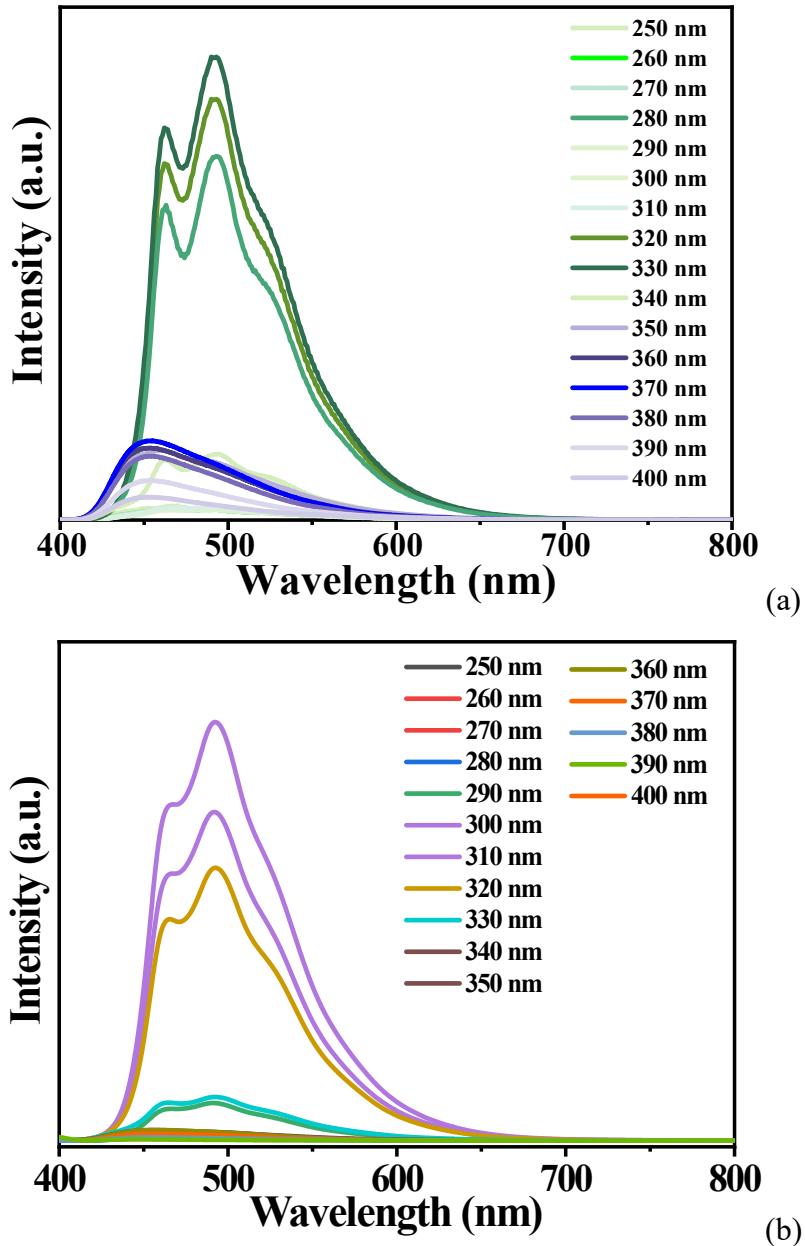


Fig. S10. The prompt-mode (a) and delayed-mode (b) excitation wavelength dependent PL emission spectra of $[BTPP]_2CdBr_4$.

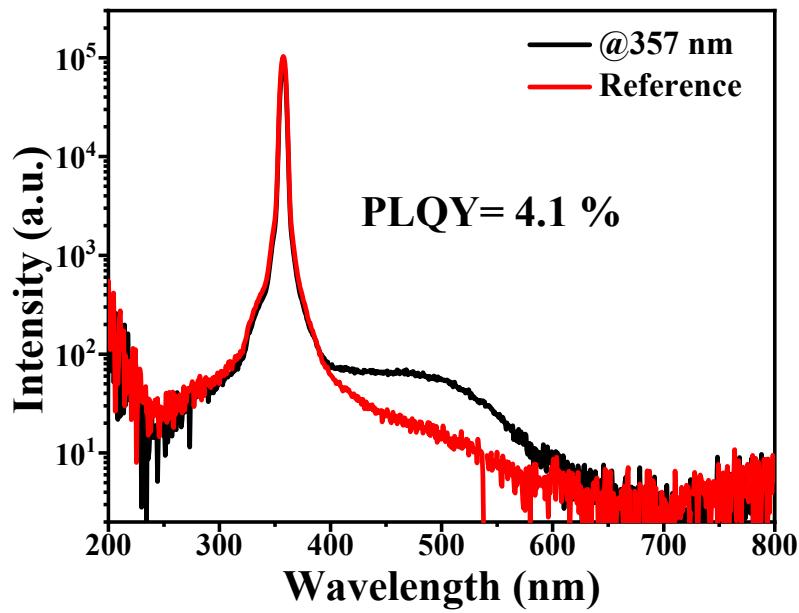


Fig. S11. The PLQY of blue light emission excited by 357 UV light for $[\text{BTPP}]_2\text{CdBr}_4$ at 300 K.

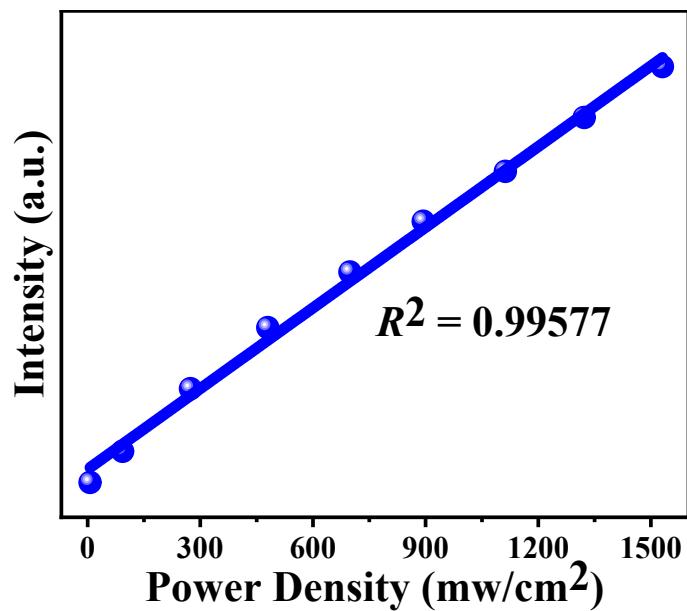


Fig. S12. The power density-dependent luminescence intensity of $[\text{BTPP}]_2\text{CdBr}_4$.

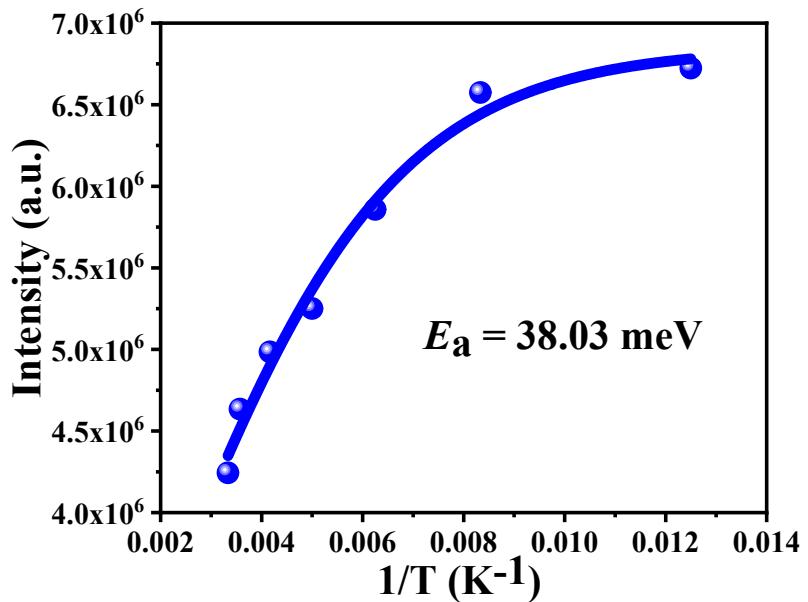


Fig. S13. Integrated PL intensity as a function of reciprocal temperature of $[\text{BTPP}]_2\text{CdBr}_4$.

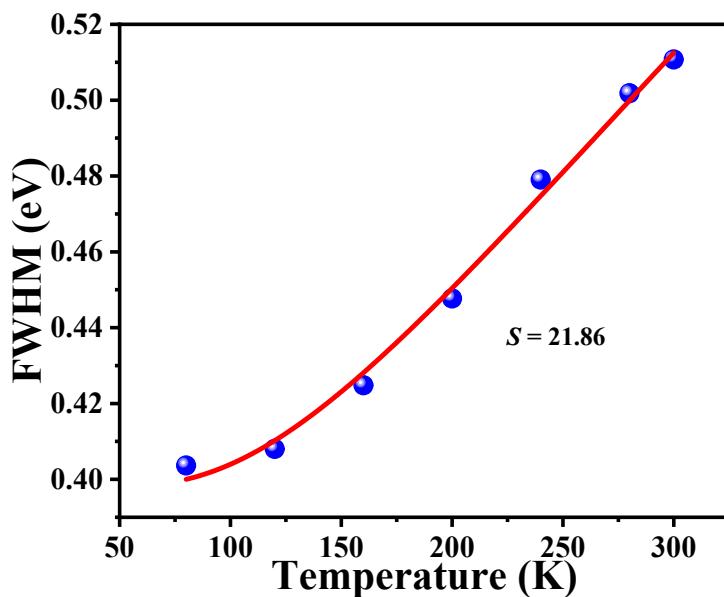


Fig. S14. Experimental and fitted temperature-dependent FWHM of $[\text{BTPP}]_2\text{CdBr}_4$.

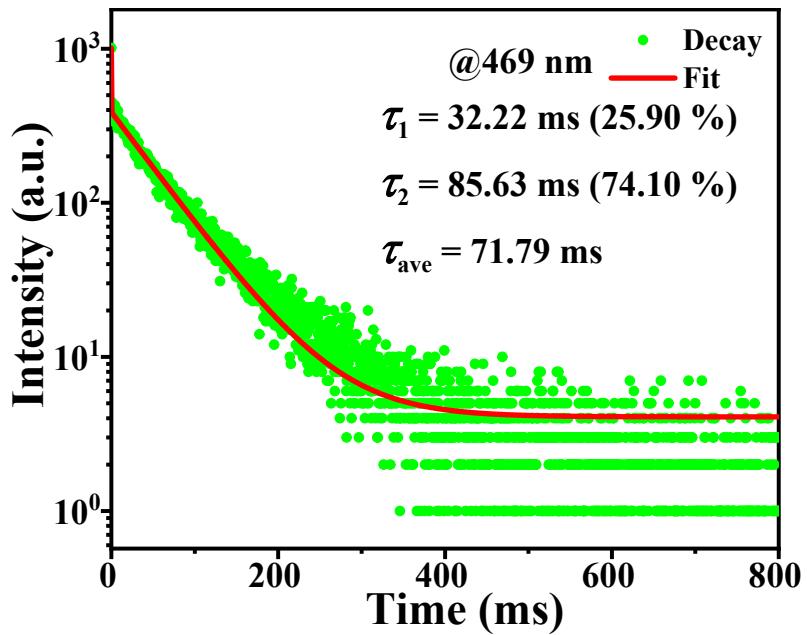


Fig. S15. PL decay curve monitoring at 469 nm excited by 309 nm for $[BTPP]_2CdBr_4$ at 300 K.

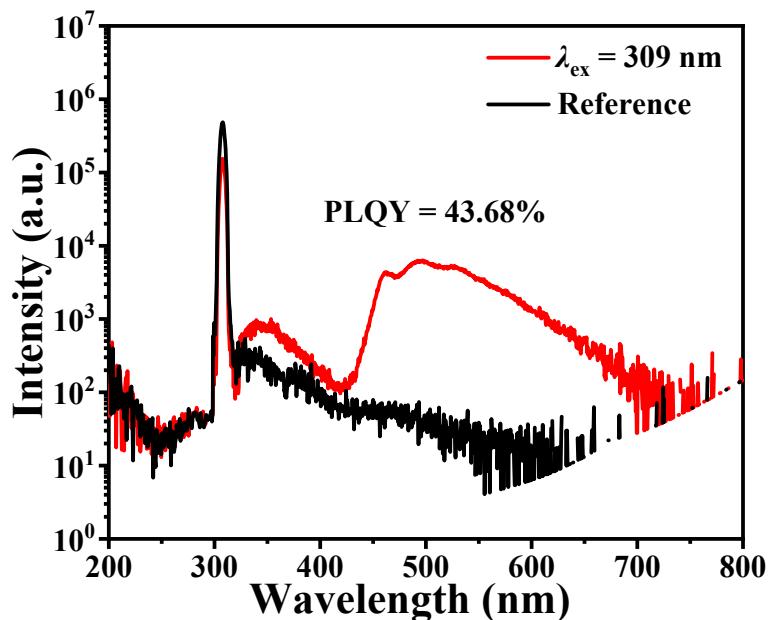


Fig. S16. The PLQY of green afterglow excited by 309 nm UV light for $[BTPP]_2CdBr_4$ at 300 K.

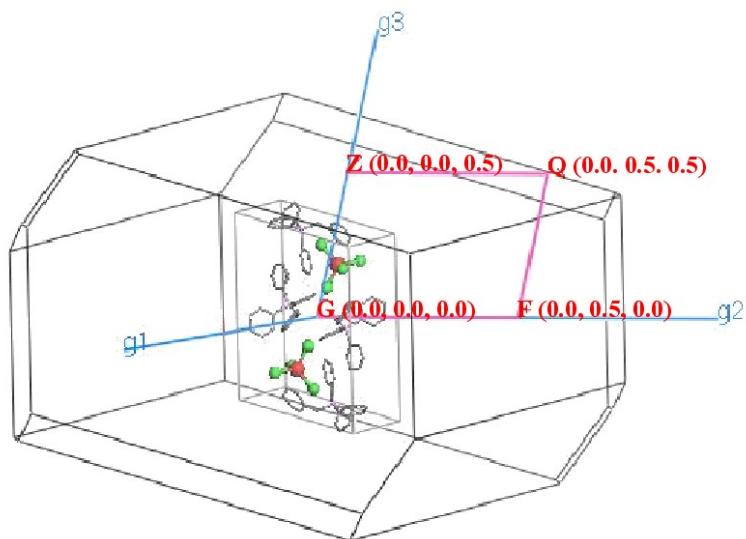


Fig. S17 The high-symmetry k points in the Brillouin zone of $[BTPP]_2CdBr_4$.

Table S1. Crystal data and structure refinement for [BTPP]₂CdBr₄.

| Compound | [BTPP] ₂ CdBr ₄ |
|---|--|
| chemical formula | C ₅₀ P ₂ H ₄₄ CdBr ₄ |
| Fw | 1138.83 |
| Space group | <i>P</i> -1 (No. 1) |
| <i>a</i> (Å) | 10.482(5) |
| <i>b</i> (Å) | 12.470(6) |
| <i>c</i> (Å) | 18.446(8) |
| α (°) | 105.694(1) |
| β (°) | 93.067(2) |
| γ (°) | 92.602(2) |
| <i>V</i> (Å ³) | 2313.3(2) |
| <i>Z</i> | 2 |
| <i>D</i> _{calcd} (g·cm ⁻³) | 1.635 |
| Temp (K) | 293 |
| μ (mm ⁻¹) | 4.029 |
| <i>F</i> (000) | 1124.0 |
| Reflections collected | 52439 |
| GOF on <i>F</i> ² | 1.024 |
| ^a <i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> >2σ(<i>I</i>)) | 0.0355/0.0652 |
| ^b <i>R</i> ₁ , <i>wR</i> ₂ (all data) | 0.0703/0.0746 |

$$^aR_1 = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad ^b wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}.$$

Table S2. Selected bond lengths (\AA) and bond angles ($^\circ$) for $[\text{BTPP}]_2\text{CdBr}_4$.

| | | | |
|-------------|------------|-------------|------------|
| Cd1-Br2 | 2.6460(11) | Cd1-Br4 | 2.5817(10) |
| Cd1-Br1 | 2.5682(9) | Cd1-Br3 | 2.5713(10) |
| Br1-Cd1-Br2 | 111.69(4) | Br4-Cd1-Br2 | 108.07(2) |
| Br1-Cd1-Br4 | 111.62(3) | Br3-Cd1-Br2 | 105.46(2) |
| Br1-Cd1-Br3 | 109.01(3) | Br3-Cd1-Br4 | 110.82(4) |

Table S3. Hydrogen bonds data for $[\text{BTPP}]_2\text{CdBr}_4$.

| D-H \cdots A | d(D-H) | d(H \cdots A) | d(D \cdots A) | \angle (DHA) |
|-----------------------|--------|-----------------|-----------------|----------------|
| C13-H13A \cdots Br2 | 0.97 | 2.89 | 3.847(4) | 170 |
| C13-H13B \cdots Br2 | 0.97 | 2.88 | 3.806(4) | 161 |
| C24-H24 \cdots Br2 | 0.93 | 2.88 | 3.793(4) | 169 |