Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Zero-dimensional Organic-inorganic Hybrid Zinc Halide with Broadband Yellow Light Emission

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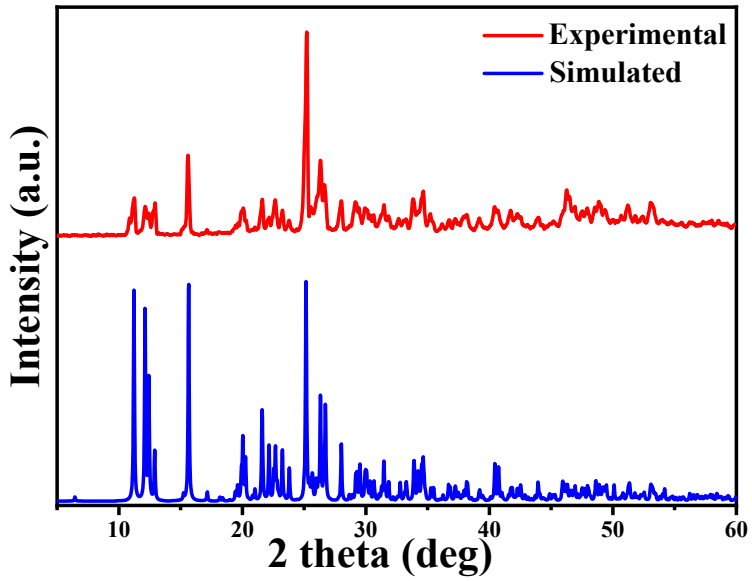


Fig. S1. The simulated and experimental power X-ray diffraction pattern of [N-EPD]$_2$ZnBr$_4$.

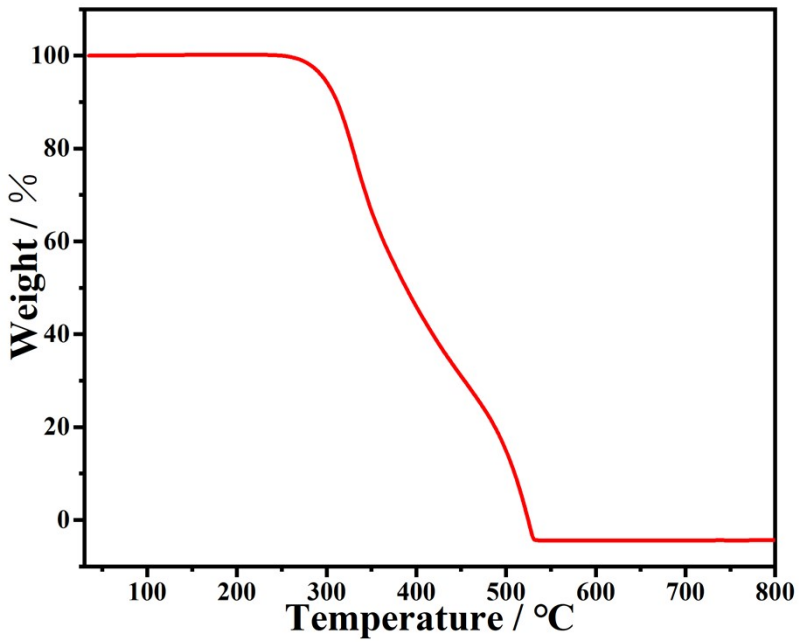


Fig. S2. The thermogravimetric analysis of [N-EPD]$_2$ZnBr$_4$.

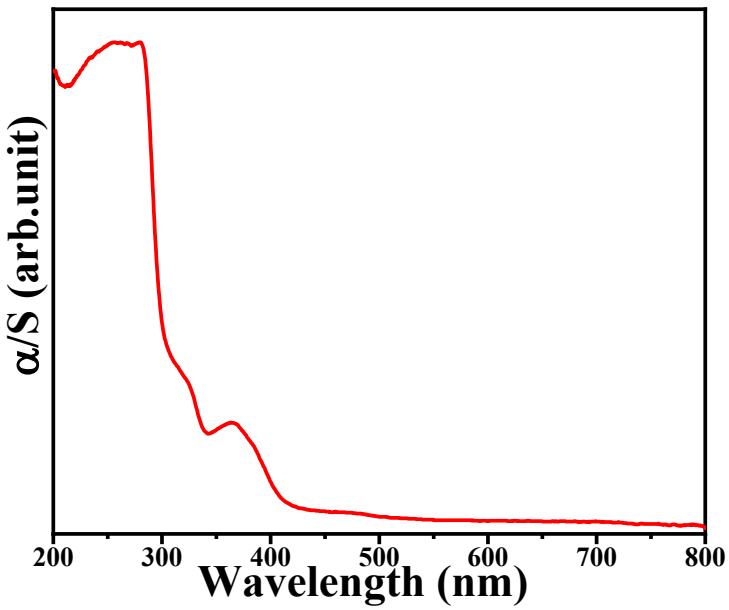


Fig. S3. The UV−vis absorption spectrum of $[N\text{-}EPD]_2ZnBr_4$.

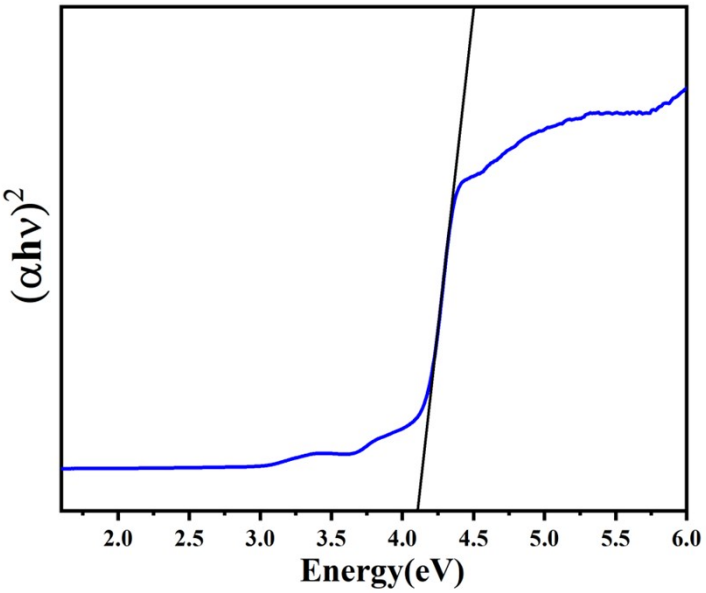


Fig. S4. The Tauc's plots for $[N\text{-}EPD]_2ZnBr_4$.

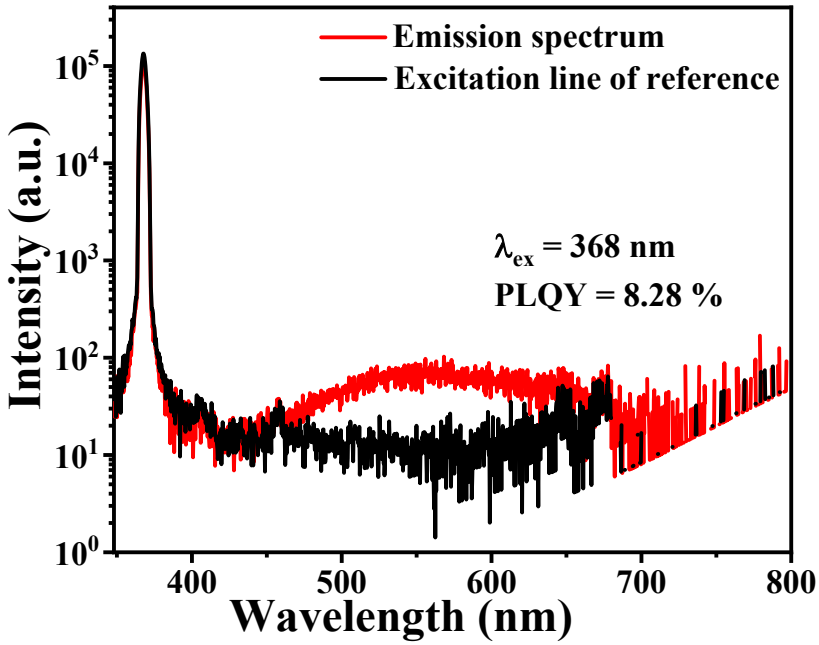
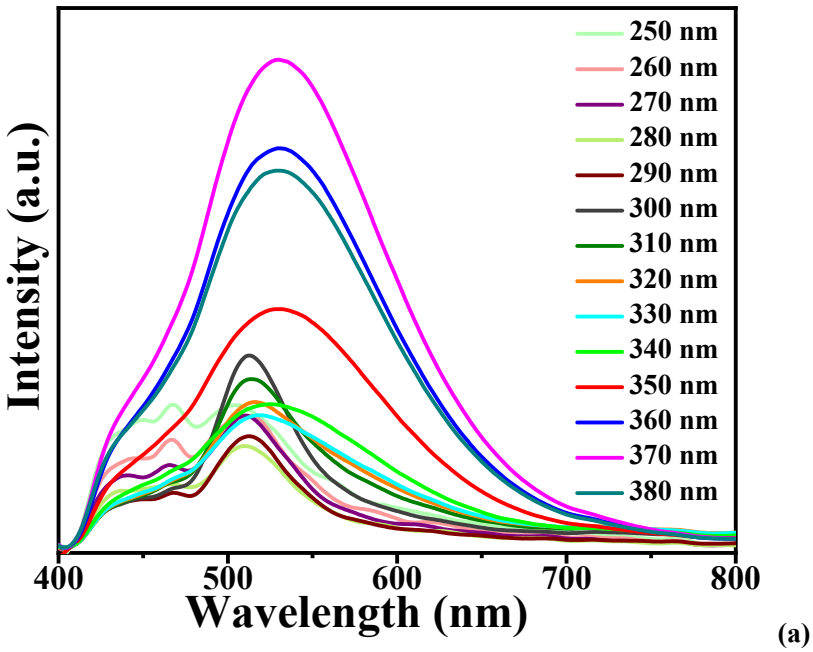
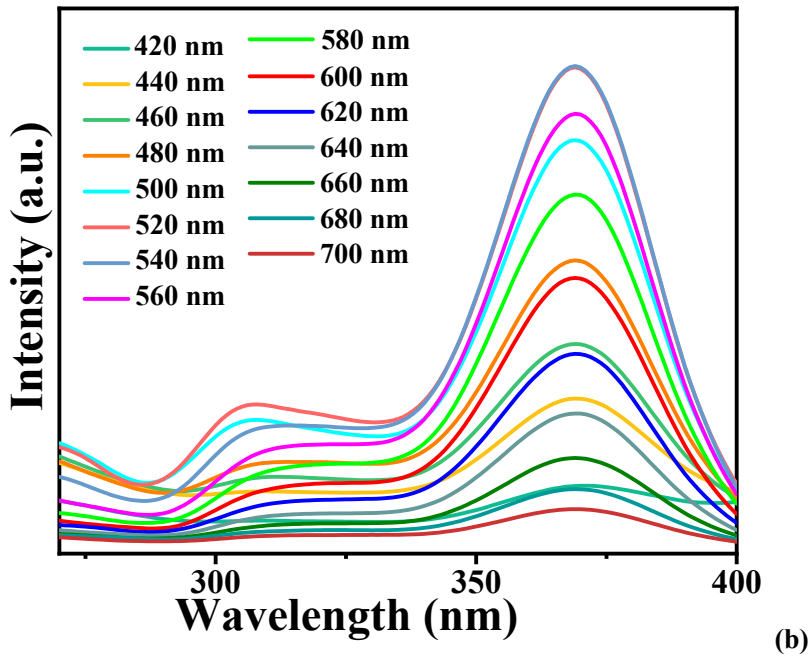


Fig. S5. The PLQY of $[N\text{-}EPD]_2ZnBr_4$ at 300K.

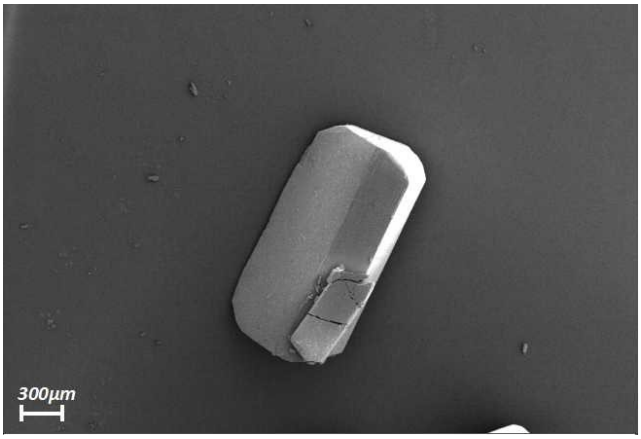


(a)

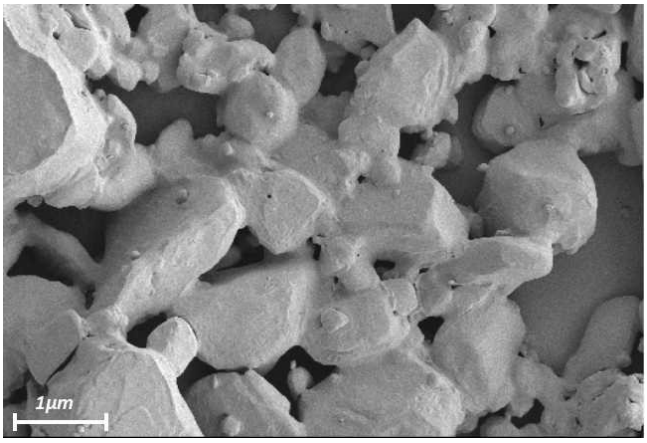


(b)

Fig. S6. The excitation wavelength dependent PL emission spectra (a) and the emission wavelength dependent PL excitation spectra (b) of $[N\text{-}EPD]_2ZnBr_4$.



(a)



(b)

Fig. S7. The SEM photos of (a) bulk crystals and (b) microscale crystals of [N-EPD]$_2$ZnBr$_4$.

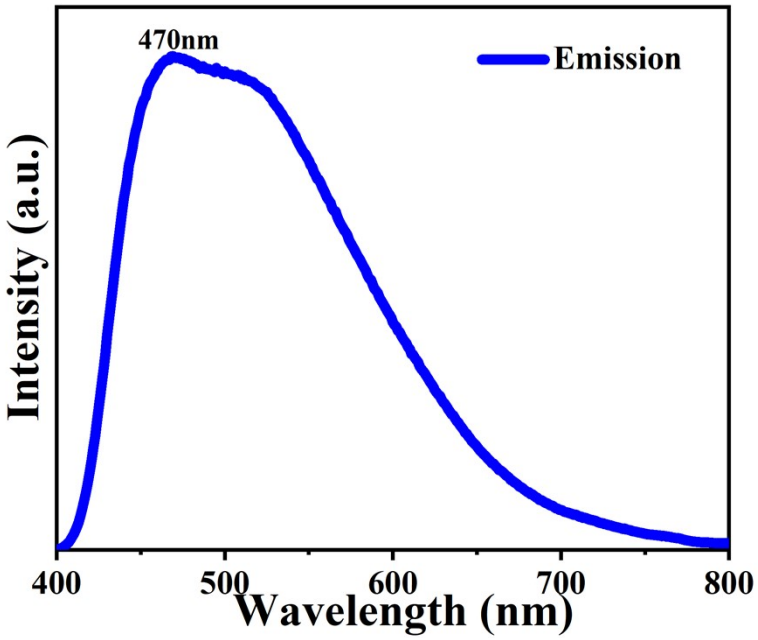


Fig. S8. PL emission spectrum of [N-EPD]Br at 300 K.

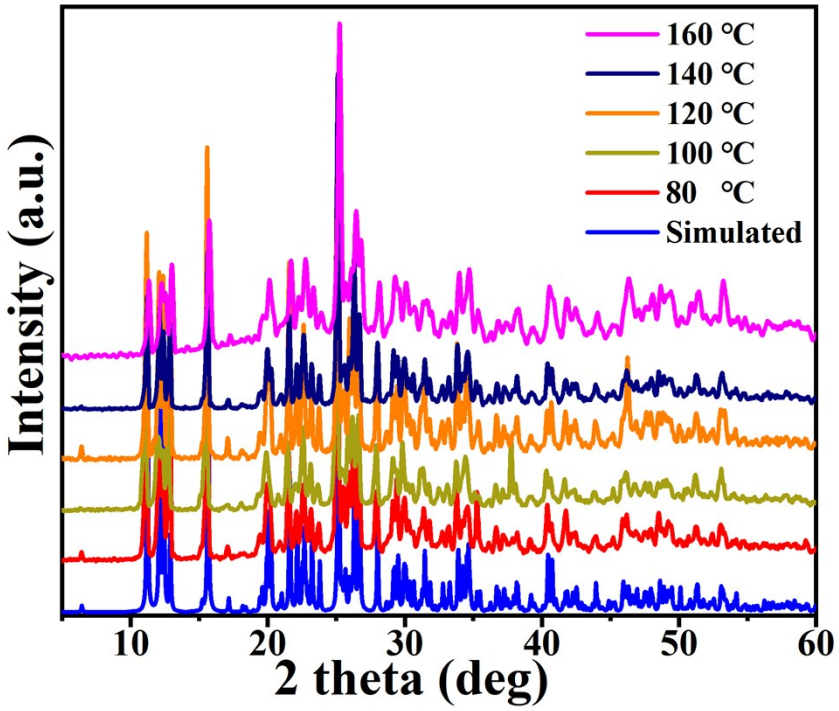


Fig. S9. The experimental PXRD patterns after continuous heating from 80 ℃ to 160 ℃.

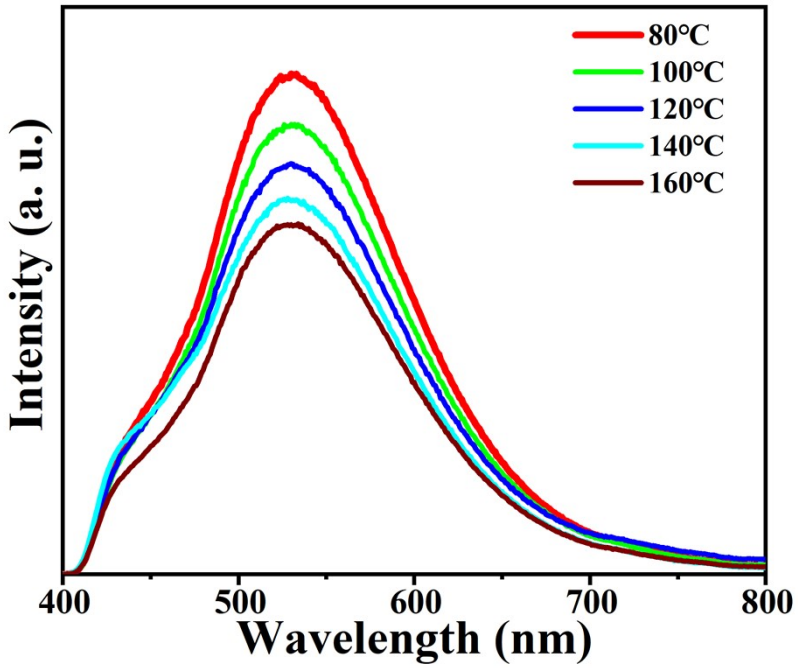


Fig. S10. The PL emission spectra of $[N\text{-}EPD]_2ZnBr_4$ after continuous heating from 80 ℃ to 160 ℃.

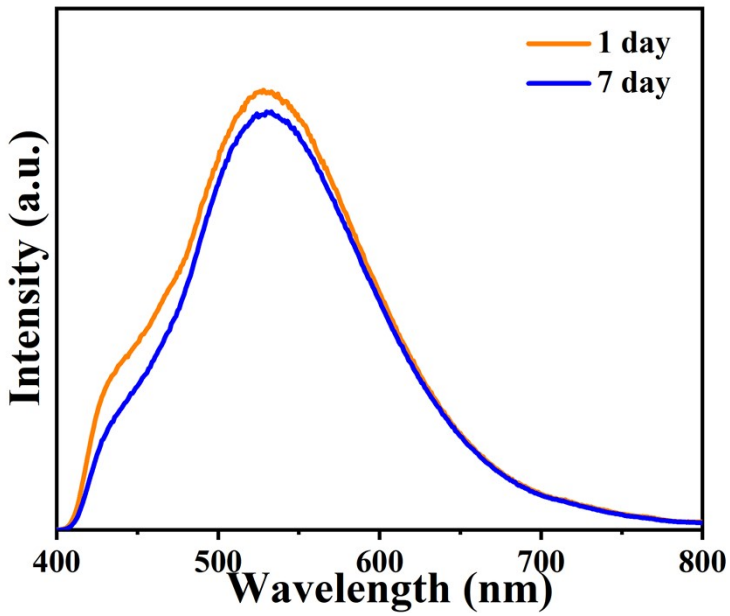


Fig. S11. The PL spectra of $[N\text{-}EPD]_2ZnBr_4$ before and after storing in ambient atmosphere with relative humidity of about 50% for one week.

Table S1. Crystal Data and Structural Refinements for $[N\text{-}EPD]_2ZnBr_4$.

Compound	$[N\text{-}EPD]_2ZnBr_4$
chemical formula	$C_{14}H_{20}N_2ZnBr_4$
fw	603.35
Space group	*C2/c*
crystal system	Monoclinic
a/Å	27.5957(4)
*b*Å	8.22990(10)
c/Å	17.9221(3)
β/º	96.3750(10)
V(Å^3)	4045.12(10)
Dcalcd (g·cm^{-3})	1.9813
Temp (K)	298.15
μ (mm^{-1})	10.899
F (000)	2288.7
Reflections collected	10486
Unique reflections	3857
GOF on F^2	1.004
[a]R_1,wR_2 ($I > 2\sigma(I)$)	0.0297/0.0833
[b]R_1,wR_2 (all data)	0.0324/0.0856
CCDC number	2208029

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [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 (Å) and bond angles (°) for compound [N-EPD]$_2$ZnBr$_4$.

Zn1-Br1	2.4296(5)	Zn1-Br2	2.4158(5)
Zn1-Br3	2.4208(5)	Zn1-Br4	2.3947(6)
Br2-Zn1-Br1	109.11(2)	Br3-Zn1-Br1	107.52(2)
Br3-Zn1-Br2	109.12(2)	Br4-Zn1-Br1	107.82(2)
Br4-Zn1-Br2	112.49(2)	Br2-Zn1-Br1	110.64(2)