Supporting information

Zero-Dimensional Cadmium Halide with Broad Band Yellow Light Emission for White Light-Emitting Diodes

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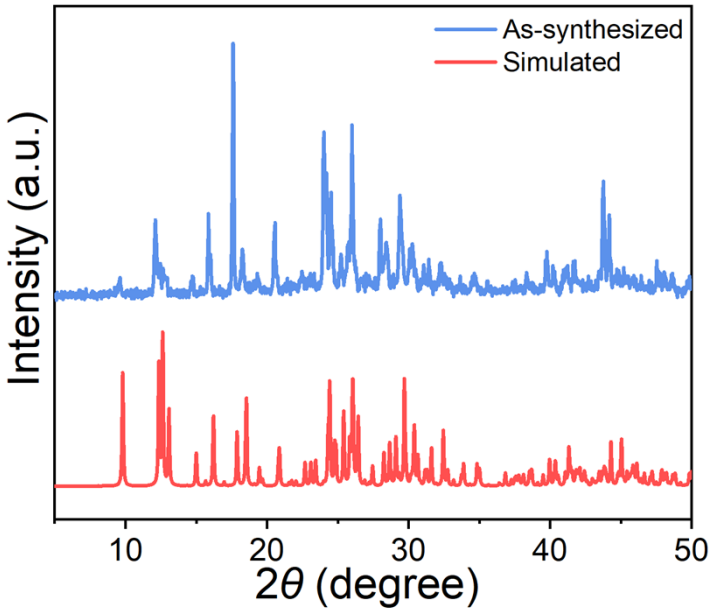


Figure S1. Powder X- ray diffraction pattern of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.

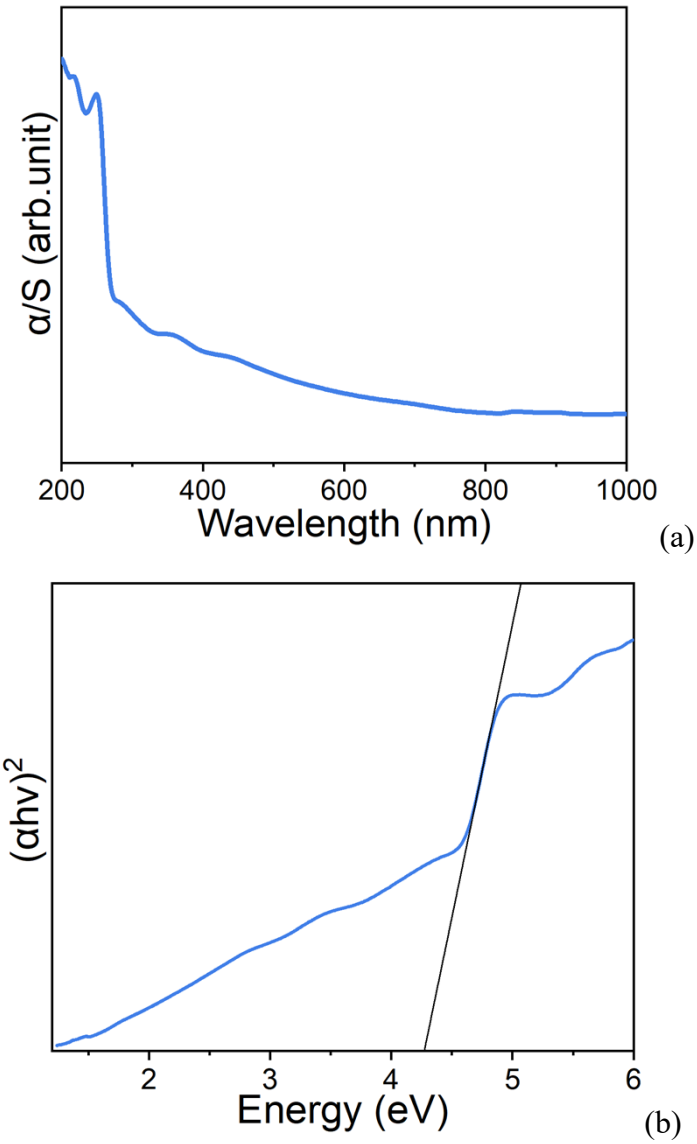
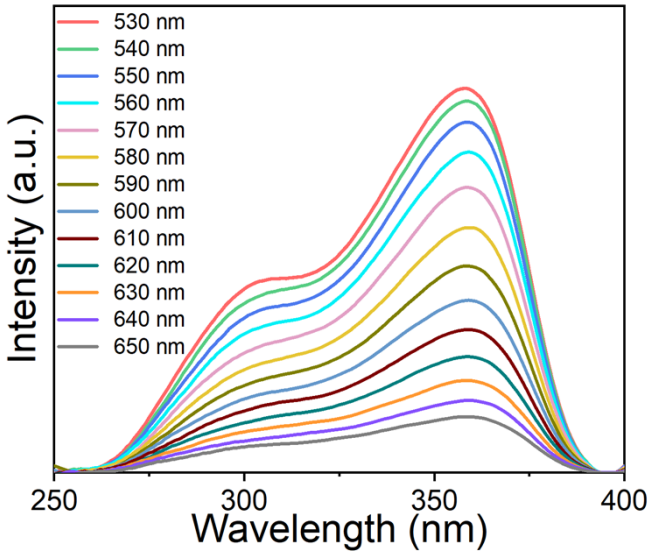
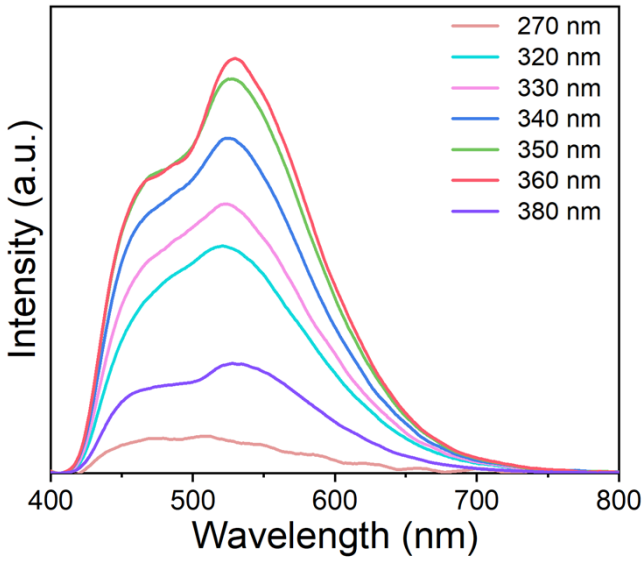


Figure S2. The solid state UV-Vis absorption optical spectrum (a) and Tauc's plots based on the assumption of indirect band gap (b) of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.



(a)



(b)

Figure S3. (a) Varied PLE spectra and (b) PL spectra of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$ at different wavelength.

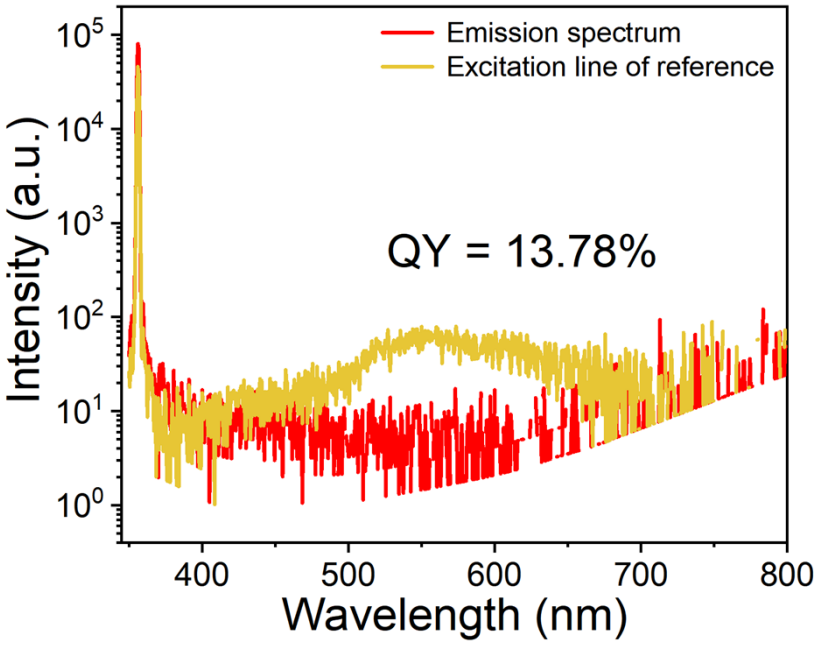


Figure S4. The PLQY spectra of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.

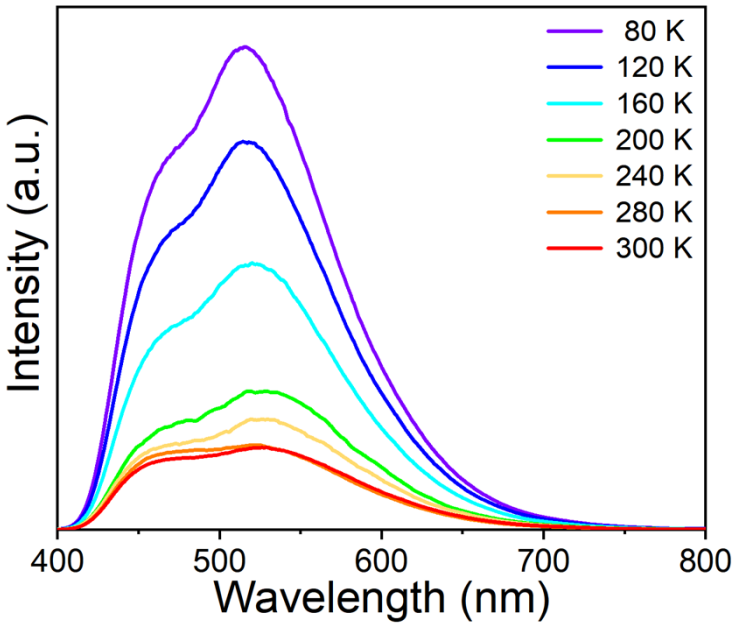


Figure S5. Temperature-dependent PL spectra of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.

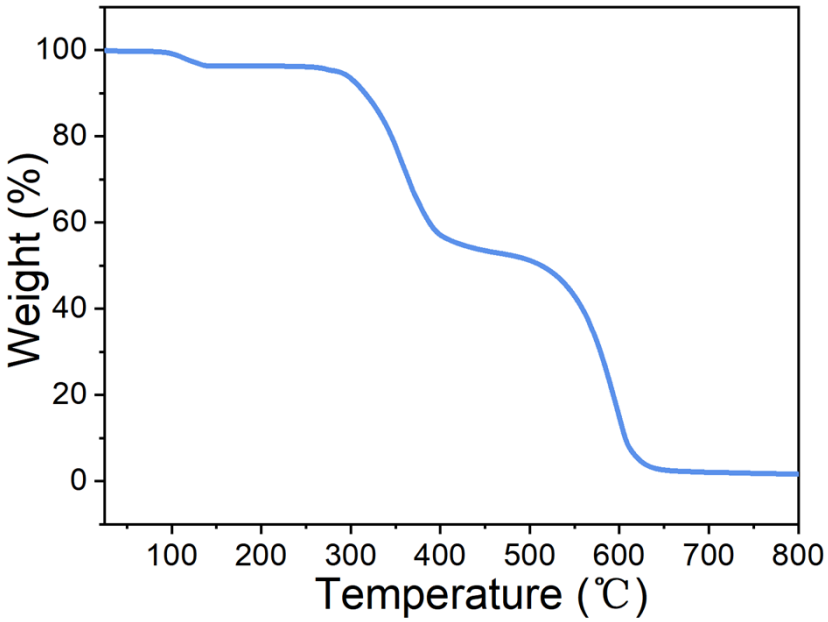
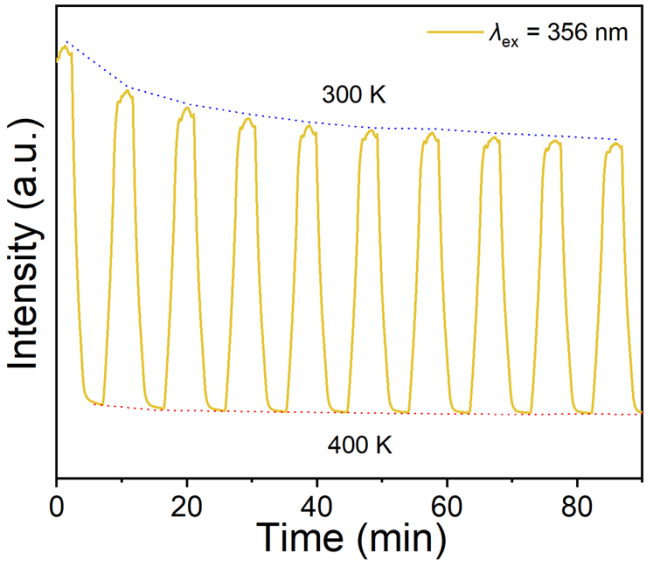
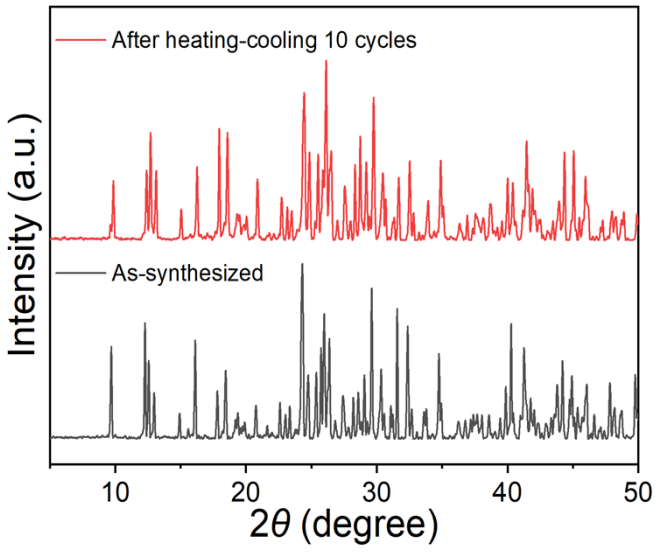


Figure S6. The thermogravimetric analyse (TGA) curves of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.



(a)



(b)

Figure S7. (a) The PL intensity investigated by heating-cooling the sample in the temperature range from 300 K to 400 K repeatedly. (b) The XRD patterns of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$ after heating-cooling 10 cycles.

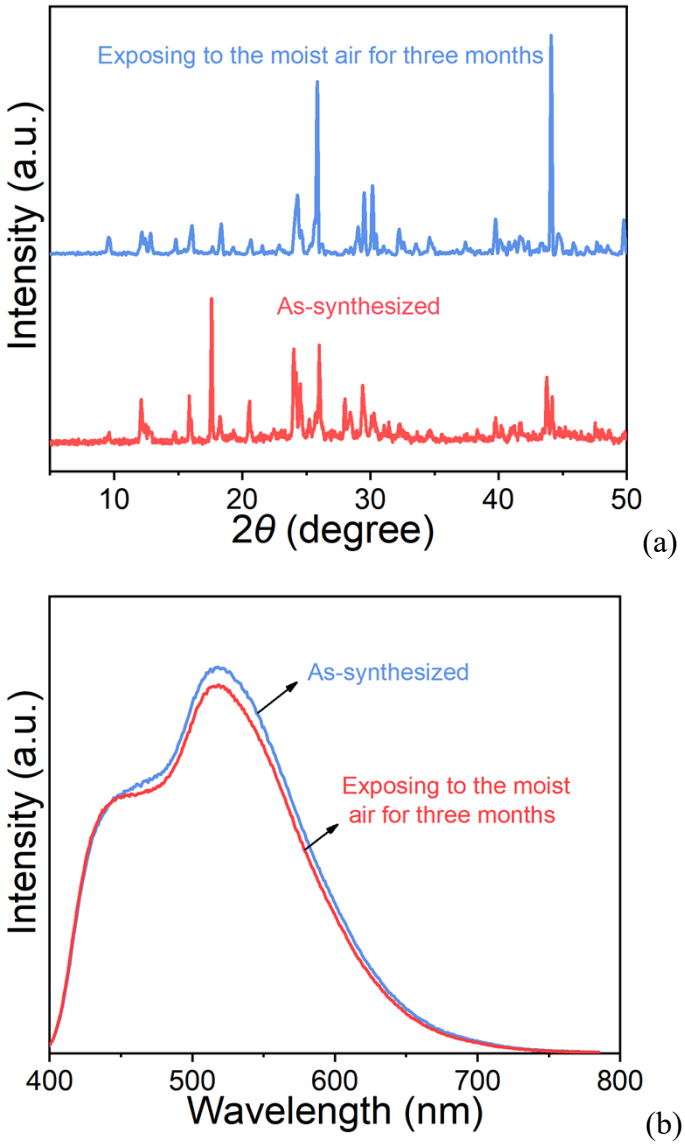
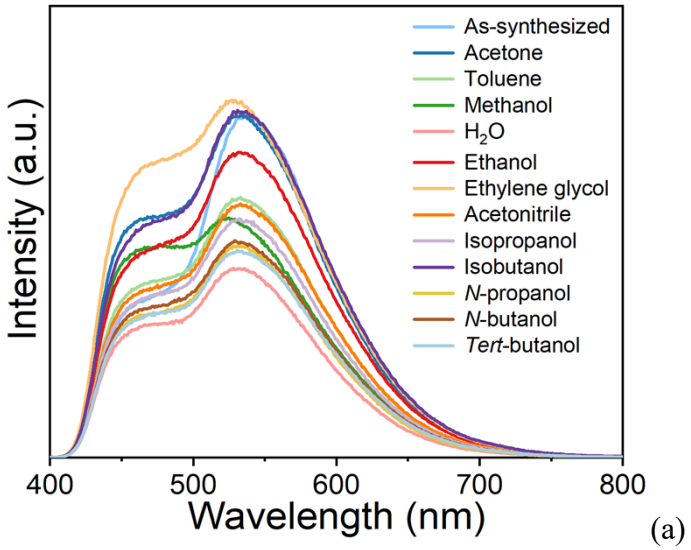
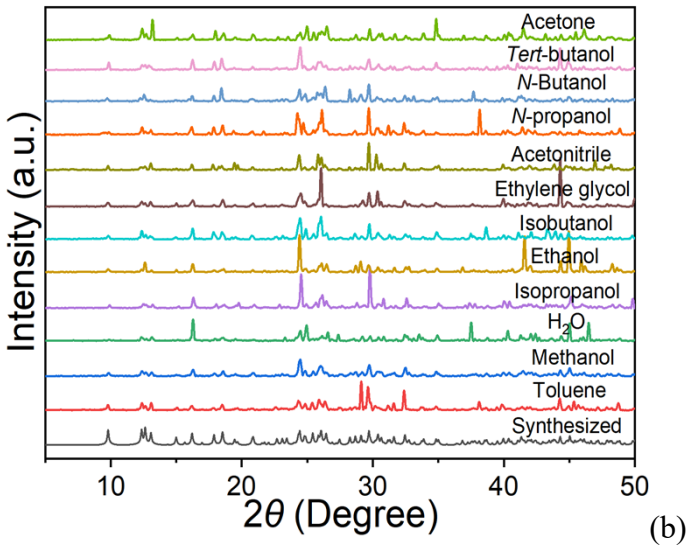


Figure S8. The PXRD pattern (a) and PL emission spectra (b) of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$ after exposing to the moist air for three months.

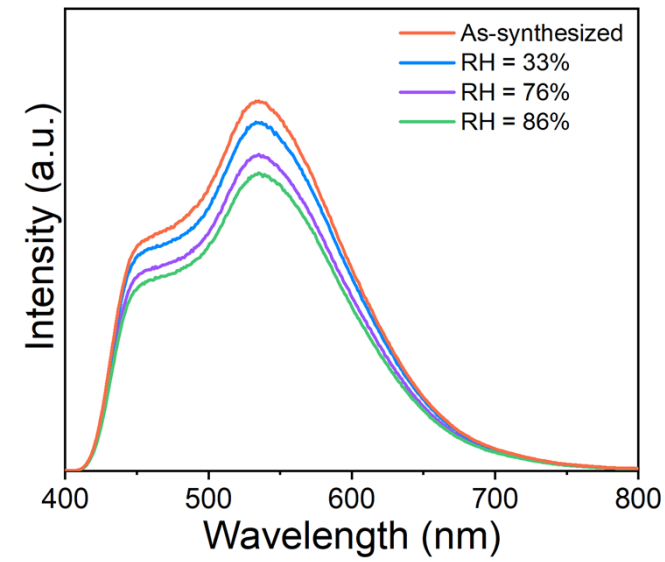


(a)

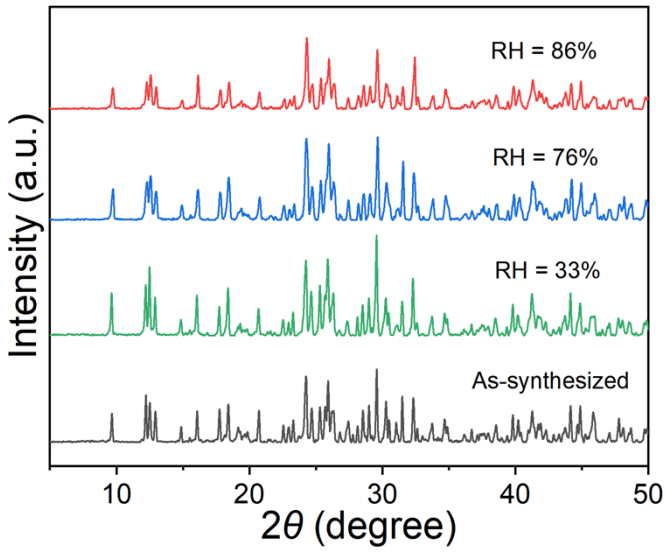


(b)

Figure S9. (a) PL emission spectra and (b) X-ray diffraction (PXRD) patterns of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$ after soaking in various organic solvents for 24 hours.

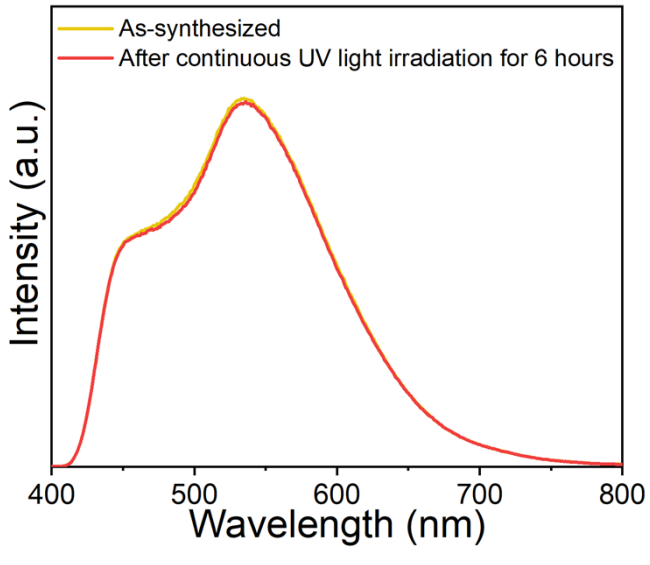


(a)

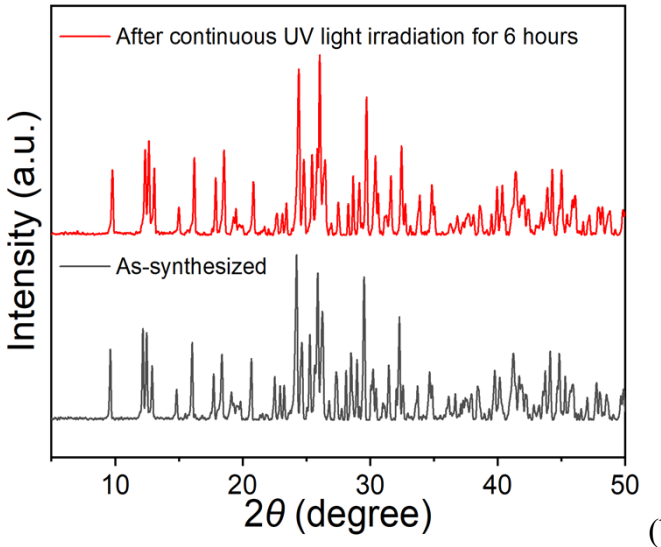


(b)

Figure S10. (a) The PL spectra and (b) X-ray diffraction (PXRD) patterns under different relative humidity of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.



(a)



(b)

Figure S11. (a) The PL spectra and (b) X-ray diffraction (PXRD) patterns under continuous UV light irradiation for over 6 hours of (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.

Table S1. Crystal Data and Structural Refinements for (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.

Compound	(BAPPz)$Cd_2Br_8 \cdot 2H_2O$
Chemical formula	$C_{10}H_{32}N_4O_2Cd_2Br_8$
FW	552.24
Space group	*P*-1
a/Å	7.0976(4)
*b*Å	9.1098(5)
c/Å	11.0003(6)
α/°	86.013(2)
β/°	84.060(2)
γ/°	82.390(2)
V(Å^3)	700.08(7)
Z	2
D_{calcd} (g·cm^{-3})	2.620
Temp (K)	273.15
μ(mm^{-1})	12.947
F(000)	512.0
Reflections collected	13809
Unique reflections	3467
GOF on F^2	1.078
[a]R_1,wR_2 ($I > 2\sigma(I)$)	0.0299/0.0730
[b]R_1,wR_2 (all data)	0.0347/0.0751

[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 (BAPPz)$Cd_2Br_8 \cdot 2H_2O$.

Bond	Length (Å)	Bond	Length (Å)
Cd(1)-Br(1)	2.5770(5)	Cd(1)-Br(2)	2.6010(16)
Cd(1)-Br(3)	2.5769(5)	Cd(1)-Br(4)	2.6430(4)
Bond angle	Degree (°)	Bond angle	Degree (°)
Br(1)-Cd(1)-Br(3)	106.43(13)	Br(3)-Cd(1)-Br(2)	111.6(6)
Br(1)-Cd(1)-Br(4)	106.02(13)	Br(3)-Cd(1)-Br(4)	109.865(14)
Br(2)-Cd(1)-Br(4)	101.30(6)		

Table S3. Summary of the properties of white LED materials.

Materials	Emission (nm)	Types of phosphors	PLQY	CRI	CCT	Reference
$(H_2DABCO)Pb_2Cl_6$	455, 585	0	2.5%	96	5393 K	*Chem. Sci.*, **2015**, *6*, 7222-7226.
$[(2\text{-mb})tpp]_2MnCl_4$	513	2	64.07%	95.4	5305 K	*Chem. Eng. J.*, **2022**, *450*, 138458.
$(DMP)CdBr_3$	432	2	52.3%	95.4	4922 K	*Mater. Today Chem.*, **2022**, *24*, 100766.
$(BAPPz)Cd_2Br_8 \cdot 2H_2O$	527	1	13.78%	93.7	6556 K	**This work**
$Rb_2Cu_2I_4(C_4H_8OS)_3$	588	1	86%	93	5465 K	*Chem. Mater.* **2023**, *35*, 1318-1324.
$Cs_3NaInCl_6 \cdot H_2O$: Sb^{3+},Bi^{3+}	450	0	99.5%	92.9	4936 K	*Laser Photonics Rev.* **2024**, 2401084.
$(C_3H_7)_4N]_2Cu_2I_4$	483	0	91.9%	92.2	5684 K	*ACS Appl. Mater. Interfaces* **2022**, *14*, 12395-12403.
ZJU28⊃DSM/AF	625	0	60.72%	91	5327	*Adv. Funct. Mater.* **2015**, *25*, 4796-4802.
$Zn(SCN)_2$-codoped $CsPbBr_3$ NCs	514	1	90%	89	6046 K	*J. Alloy. Compd.* **2024**, *1005*, 176064.
$(H_3O)(Et_2\text{-}DABCO)_8Pb_{21}Cl_{59}$	420, 690	0	1%	88	3496 K	*Chem. Sci.*, **2015**, *6*, 7222-7226.
$(C_{25}H_{22}P)_2SbCl_5$	593	1	98.6%	87	4000 K	*ACS Appl. Mater. Interfaces* **2022**, *14*, 45611-45620.
$(C_{19}H_{18}P)_2Cu_4I_6$	620	0	87.4%	86.7	5233 K	*Adv. Optical Mater.* **2024**, *12*, 2401050.
$CsBr/Eu^{2+}$ nanocrystal	447	2	55.8%	85.6	3920 K	*ACS Appl. Nano Mater.* **2024**, *7*, 20145-20152.
$Cs_2Ag_{0.80}K_{0.20}In_{0.875}Bi_{0.125}Cl_6$	629	1	15.96%	85	3878 K	*J. Alloy. Compd.* **2023**, *960*, 170836.
$InCl_3$-TPOBD	547	0	10.5%	84.8	9370 K	*Adv. Funct. Mater.* **2023**, *33*, 2214962.
$PPASnCl_6$:3.5%Sb	660	2	77%	84	5863 K	*Adv. Optical Mater.* **2021**, *9*, 2101637.

$Mn@C_4H_{12}N_2ZnBr_4$	518	2	99.1%	83.3	5811 K	*Chem. Eng. J.*, **2023**, *468*, 143818.
$(HMEDA)CdBr_4$	445	0	~1%	83	10536 K	*Chem Asian J.* **2020**, *15*, 3050-3058.
$[Cu_4I_4(Ph_3As)_3]$	565	0	100%	82	6000 K	*Adv. Optical Mater.* **2024**, *12*, 2302904.
$(C_9NH_{20})_9[Pb_3Br_{11}](MnBr_4)_2$	565, 528	1	49.8%	79	6022 K	*Angew. Chem., Int. Ed.* **2019**, *58*, 18670-18675.
$K(La_{0.98}Bi_{0.02})Ta_2O_7$	550	1	42.3%	77.8	6710	*ACS Appl. Mater. Interfaces* **2018**, *10*, 24648-24655.
$[Pb_2Cl_2^{2+}][3,5\text{-}pdc^{2-}]$	411	1	72%	70	5534 K	*Adv. Optical Mater.* **2022**, *10*, 2102148.