Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Exceptional Optical Performance of Zero-Dimensional Hybrid Cuprous Halide $ETPA_2Cu_2I_4$ as an X-ray Scintillator

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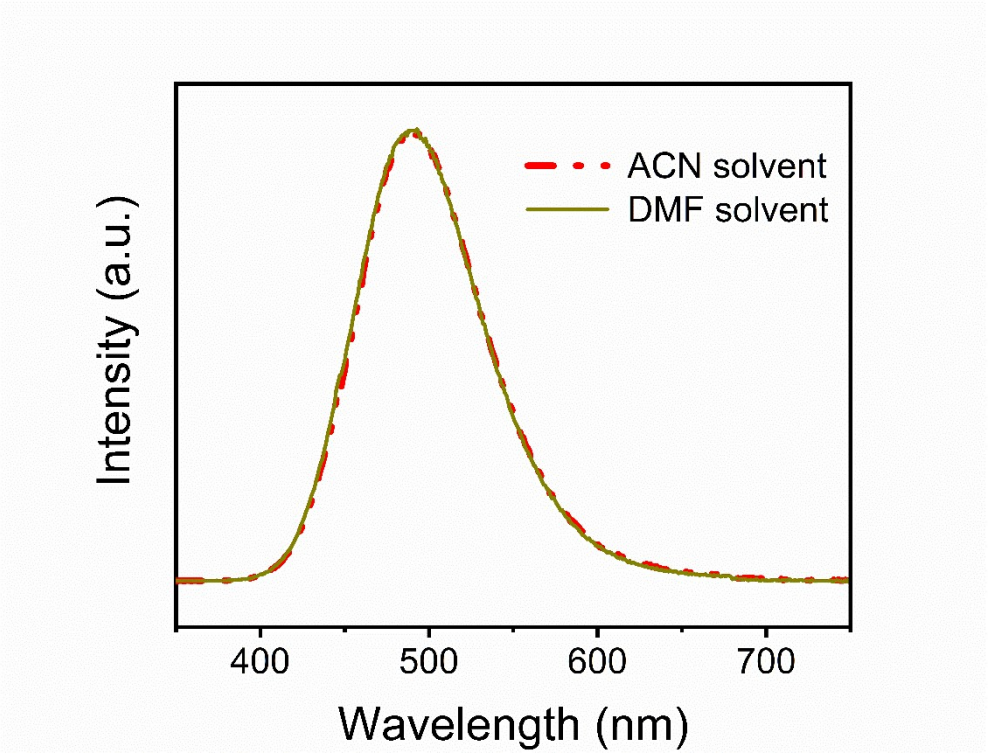

Figure S1. The PL spectra of powder synthesized with acetonitrile (CAN) and DMF were compared.

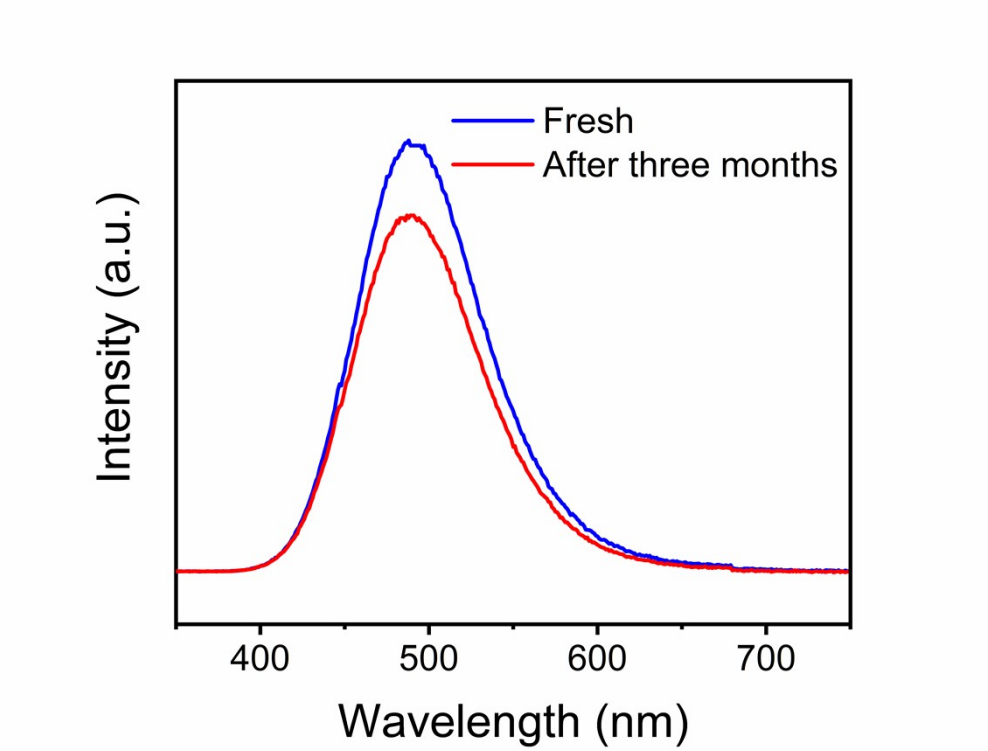

Figure S2. Comparison of PL spectra of samples after three months at constant humidity and spectra of freshly prepared samples.

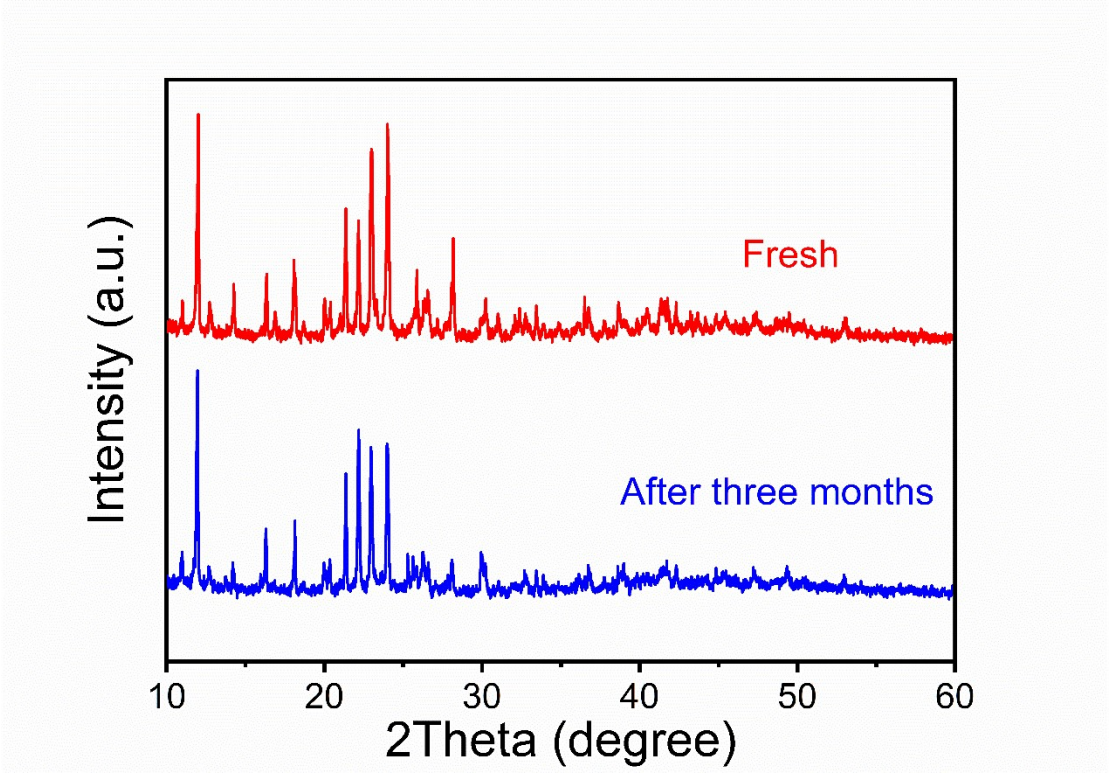

Figure S3. After standing at constant humidity for three months, the PXRD of the sample and the newly prepared sample were compared.

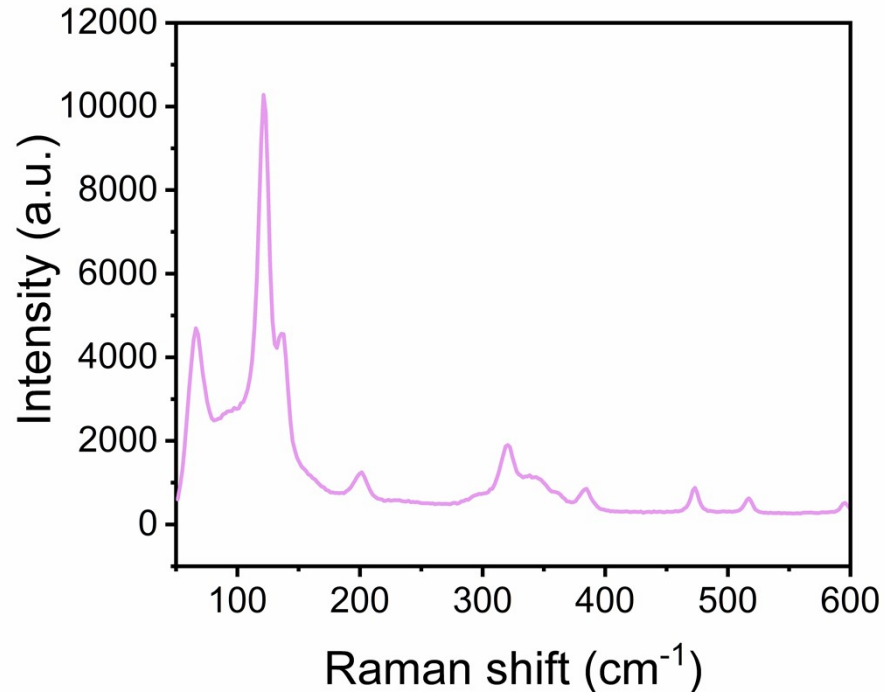

Figure S4. The Raman spectrum for $ETPA_2Cu_2I_4$ power.

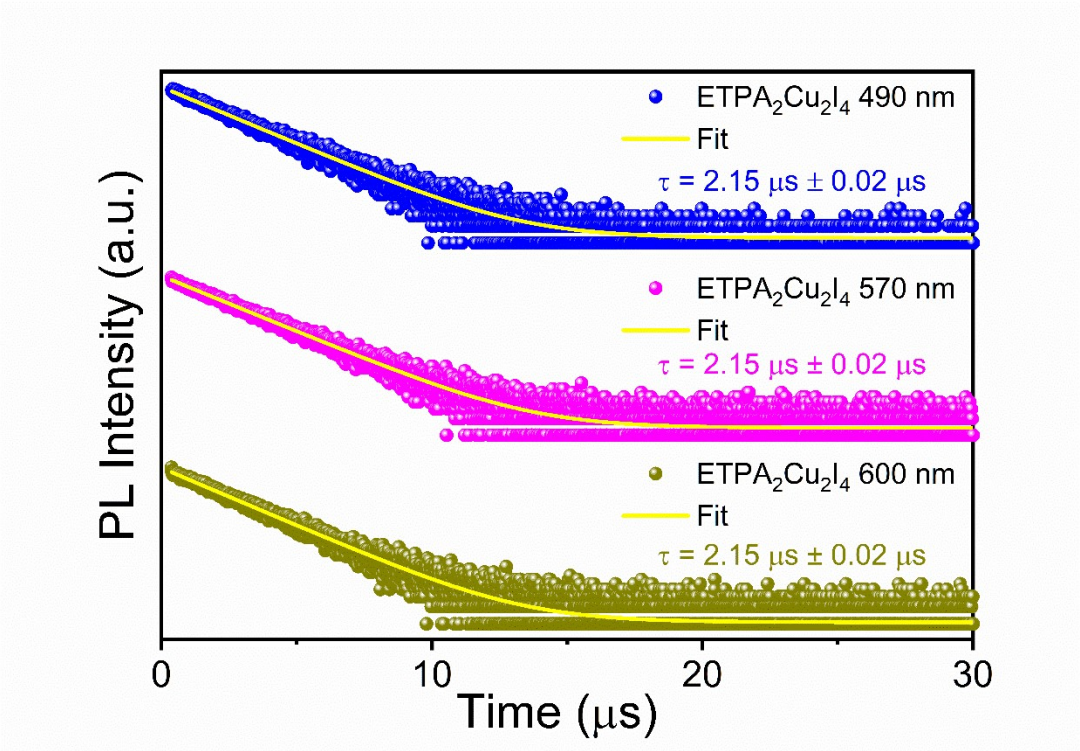

Figure S5. The lifetime comparison of different emission wavelengths of the band emission is measured.

Table S1. The element ratio in SEM images of $ETPA_2Cu_2I_4$ single crystal.

Spectrum				
Element	Line type	Weight%	Wt % Sigma	Atomic%
C	K	31.34	0.14	79.04
Cu	L	19.20	0.13	9.15
I	L	49.46	0.14	11.81
N	K	0.00	0.28	0.00
Totals	/	100.00	/	100.00

Table S2. The crystal structure parameters of $ETPA_2Cu_2I_4$ single crystals.

Compound	$[C_{11}H_{26}N]_2Cu_2I_4$
Empirical formula	$C_{11}H_{26}CuI_2N$
Formula weight	489.67
Temperature/K	193
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.7432(4)
b/Å	13.7442(4)
c/Å	14.1671(5)
α/°	90
β/°	99.9180(10)
γ/°	90
V/Å^3	1676.99(11)
Z	4
Dcalcd (g/cm^3)	1.939
μ (mm^{-1})	4.962
F (000)	936
Radiation	MoKα (λ = 0.71073)
Reflections collected	15272
Independent reflections	3826
Goodness-of-fit on F^2	1.038
Final R indexes (I>2σ(I))	R_1[a] = 0.0430, wR_2 = 0.1080
Final R indexes (all data)	R_1 = 0.0511, wR_2[b] = 0.1145

[a] $R_1 = \sum \| Fo | - | Fc \| / \sum | Fo |$, [b] $wR_2 = [\sum w(F_o^2 - F_c^2)2 / \sum w(F_o^2)^2]^{1/2}$

Table S3. Main bond lengths in $ETPA_2Cu_2I_4$ single crystals.

Atom	Atom	Length/Å
I1	Cu1	2.4917(7)
I2	Cu11	2.5604(8)
I2	Cu1	2.5503(8)
Cu1	Cu11	2.8560(13)
N1	C4	1.516(6)
N1	C1	1.511(6)
N1	C10	1.514(7)
N1	C7	1.534(7)
C4	C5	1.501(8)
C1	C2	1.496(9)
C10	C11	1.481(9)
C5	C6	1.482(9)
C7	C8	1.468(9)
C2	C3	1.485(8)
C8	C9	1.468(10)

Table S4. Main bond angles in $ETPA_2Cu_2I_4$ single crystals.

Atom	Atom	Atom	Angle/°
Cu1	I2	Cu11	67.95(3)
I1	Cu1	I2	125.35(3)
I1	Cu1	I21	122.56(3)
I1	Cu1	Cu11	177.55(4)
I2	Cu1	I21	112.05(3)
I2	Cu1	Cu11	56.19(2)
I21	Cu1	Cu11	55.86(2)
C4	N1	C7	108.8(4)
C1	N1	C4	108.8(4)
C1	N1	C10	109.7(4)
C1	N1	C7	110.7(4)
C10	N1	C4	111.1(4)
C10	N1	C7	107.8(4)
C5	C4	N1	116.8(5)
C2	C1	N1	116.6(5)
C11	C10	N1	117.6(5)
C6	C5	C4	111.5(6)
C8	C7	N1	116.9(5)
C3	C2	C1	113.1(6)
C9	C8	C7	115.1(7)

Table S5. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $ETPA_2Cu_2I_4$ single crystals. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
I1	9445.2(5)	4057.6(3)	7529.8(3)	58.44(17)
I2	11379.3(6)	6172.6(3)	5636.7(3)	68.49(18)
Cu1	9785.5(8)	4682.7(5)	5928.1(5)	52.4(2)
N1	5921(4)	7451(3)	3996(3)	40.3(8)
C4	5161(6)	7157(4)	2994(4)	51.0(11)
C1	5130(7)	8356(4)	4280(4)	55.2(13)
C10	7637(7)	7647(5)	4043(4)	62.8(15)
C5	5891(8)	6327(5)	2543(4)	64.4(15)
C7	5759(8)	6611(4)	4685(4)	57.9(13)
C11	8089(8)	8376(6)	3372(5)	80(2)
C6	5008(8)	6087(5)	1582(5)	70.3(18)
C2	3455(8)	8260(5)	4364(6)	73.4(19)
C8	6310(11)	6791(6)	5709(5)	86(2)
C3	2778(9)	9178(5)	4663(5)	73.3(19)
C9	6094(11)	5978(6)	6346(6)	95(3)

Table S6. Anisotropic displacement parameters (×10^4) for $ETPA_2Cu_2I_4$ single crystals. The anisotropic displacement factor exponent takes the form: $-2p^2$ [h^2 a*^{2} × U_{11}+ ... +2$h$ka* × b* × U_{12}]

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I1	58.4(3)	72.7(3)	47.3(2)	10.35(15)	17.78(16)	5.60(16)
I2	87.5(3)	72.1(3)	46.7(2)	1.83(16)	13.98(19)	-23.8(2)
Cu1	51.7(4)	58.1(4)	50.1(4)	7.1(3)	16.5(3)	10.0(3)
N1	39(2)	40.7(19)	40(2)	-2.2(15)	4.2(15)	-0.1(15)
C4	48(3)	57(3)	47(3)	-4(2)	6(2)	-4(2)
C1	65(3)	45(3)	55(3)	-5(2)	9(2)	0(2)
C10	50(3)	81(4)	55(3)	-8(3)	0(2)	-4(3)
C5	68(4)	71(4)	54(3)	-10(3)	12(3)	0(3)
C7	70(4)	50(3)	53(3)	3(2)	11(3)	7(3)
C11	65(4)	98(5)	78(5)	-6(4)	19(3)	-29(4)
C6	66(4)	81(4)	66(4)	-31(3)	18(3)	-15(3)
C2	74(4)	59(3)	96(5)	3(3)	39(4)	7(3)
C8	114(7)	93(5)	53(4)	18(3)	19(4)	14(4)
C3	89(5)	71(4)	67(4)	14(3)	32(3)	32(3)
C9	114(7)	103(6)	69(5)	34(4)	22(4)	46(5)

Table S7. Hydrogen fractional atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2 ×10^3) for $[C_{11}H_{26}N]_2Cu_2I_4$ single crystals. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}

Atom	x	y	z	U_{eq}
H4A	4067	6982.76	3011.23	61
H4B	5147.71	7731.49	2571.38	61
H1A	5706.37	8583.39	4904.12	66
H1B	5220.38	8869.85	3802.27	66
H10A	8068.14	7858.95	4703.58	75
H10B	8145.32	7023.92	3932.8	75
H5A	6968.8	6502.73	2485.68	77
H5B	5931.82	5747.68	2961.87	77
H7A	4649.13	6427.75	4600.81	69
H7B	6331.08	6043.77	4492.18	69
H11A	7718.98	8166.38	2711.44	120
H11B	9222.34	8438.63	3480.34	120
H11C	7624.77	9006.58	3481.38	120
H6A	5023.81	6646.37	1154.53	105
H6B	3932.1	5932.28	1634.82	105
H6C	5485.25	5525.09	1321.94	105
H2A	2859.09	8054.3	3736.96	88

H2B	3347.14	7745.24	4836.11	88
H8A	7429.54	6951.82	5801.79	104
H8B	5759.86	7366.85	5903.7	104
H3A	2875.46	9690.82	4196.69	110
H3B	3333.49	9371.84	5295.49	110
H3C	1678.49	9075.44	4694.04	110
H9A	6483.39	5377.33	6099.54	142
H9B	4987.53	5905.64	6372.25	142
H9C	6668.13	6109.5	6990.31	142