Supporting Information

Efficient and Stable Deep-Blue Emission from Lead-Free $(TEA)_2Cu_2Br_4$ for White LEDs

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Table S1. Crystal data and structure refinement

Crystallographic name/unit	Crystallographic parameters
Empirical formula	$(C_8H_{20}N)_2Cu_2Br_4$
Temperature/K	293
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.3530（16）
b/Å	13.758（3）
c/Å	11.058（2）
α/°	90
β/°	97.019（8）
γ°	90
Volume/Å	1261.3（5）
Z	2
ρ_{calc} g/cm3	1.862
μ/mm^{-1}	8.025
F（000）	696.0
Crystal size/mm^3	0.13×0.12×0.09
Radiation	MoKα（λ=0.711）
2θ range for data collection/°	4.748 to 55.052
Index ranges	-10≤h≤10,-17≤k≤17,-14≤l≤14
Reflections collected	30114
Independent reflections	2882[R_{int}= 0.0915, R_{sigma} = 0.0525]
Data/restraints/parameters	2882/0/114
Goodness-of-fit on F^2	1.044
Final R indexes [l>=2σ (l)]	R_1= 0.0453,wR_2= 0.1132
Final R indexes [all data]	R1=0.0628,wR_2=0.1305
Largest diff. peak/hole/e $\tilde{A}^{-3}$	1.16/-1.04

Table S2. Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103)

Atom	X	Y	Z	U(eq)
Br1	7338.6(7)	6010.8(4)	7864.1(5)	53.2(2)
Br2	6317.4(8)	3829.6(4)	5181.7(5)	61.9(2)
Cu1	5940.9(10)	5420.4(6)	6076.9(6)	66.9(3)
N1	1808(5)	4168(3)	7887(3)	38.0(8)
C1	3551(6)	3900(4)	7777(5)	51.3(12)
C2	4606(7)	3728(5)	8956(6)	67.7(16)
C3	960(6)	4378(4)	6614(4)	45.5(11)
C4	909(8)	3543(4)	5736(5)	60.4(14
C5	1012(6)	3333(3)	8474(4)	43.6(10)
C6	-793(7)	3397(4)	8449(5)	54.7(13)
C7	1689(6)	5069(4)	8670(4)	45.8(11)
C8	2469(8)	5970(4)	8252(6)	59.7(14)

Table S3. Anisotropic Displacement Parameters (Å2×103)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	56.8(4)	53.3(3)	47.7(3)	0.7(2)	-0.7(2)	-1.9(2)
Br2	64.0(4)	65.8(4)	53.9(4)	-3.5(3)	-0.8(3)	6.5(3)
Cu1	64.9(5)	89.7(6)	46.5(4)	-0.7(3)	8.1(3)	-20.8(4)
N1	43(2)	39.8(19)	32.1(18)	0.0(15)	6.5(15)	3.0(16)
C1	43(3)	60(3)	54(3)	0(2)	16(2)	8(2)
C2	51(3)	77(4)	72(4)	-1(3)	-4(3)	10(3)
C3	53(3)	51(3)	31(2)	4.4(19)	1(2)	4(2)
C4	77(4)	62(30	40(3)	-10(2)	-1(3)	5(3)
C5	54(3)	40(2)	37 (2)	6.5(18)	7(2)	2(2)
C6	55(3)	53(3)	59(3)	7(2)	14(2)	-2(2)
C7	53(3)	46(3)	38 (2)	-5(2)	5(2)	4(2)
C8	75(4)	47(3)	57(3)	-3(2)	4(3)	-11(3)

Table S4. Bond Lengths

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	Cu1	2.3162(10)	N1	C5	1.513(6)
Br2	Cu1[1]	2.4327(11)	N1	C7	1.523(6)
Br2	Cu1	2.4383(11)	C1	C2	1.500(8)
Cu1	Cu1[1]	2.9267(15)	C3	C4	1.501(7)
N1	C1	1.521(6)	C5	C6	1.507(7)
N1	C3	1.524(6)	C7	C8	1.500(7)

Table S5. Bond Angles

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cu1[1]	Br2	Cu1	73.86(3)	C5	N1	C1	109.0(4)
Br1	Cu1	Br2	125.77(4)	C5	N1	C3	111.2(4)
Br1	Cu1	Br2[1]	127.89(4)	C5	N1	C7	108.1(3)
Br1	Cu1	Cu1[1]	175.96(5)	C7	N1	C3	108.4(4)
Br2[1]	Cu1	Br2	106.14(3)	C2	C1	N1	115.8(4)
Br2[1]	Cu1	Cu1[1]	53.16(3)	C4	C3	N1	115.1(4)
Br2	Cu1	Cu1[1]	52.98(3)	C6	C5	N1	116.0(4)
C1	N1	C3	108.3(4)	C8	C7	N1	115.9(4)
C1	N1	C7	111.8(4)				

Table S6. Torsion Angles

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	N1	C3	C4	60.9(6)	C5	N1	C1	C2	-62.5(6)
C1	N1	C5	C6	-169.4(4)	C5	N1	C3	C4	-58.9(5)
C1	N1	C7	C8	57.9(6)	C5	N1	C7	C8	178.0(4)
C3	N1	C1	C2	176.4(5)	C7	N1	C1	C2	57.0(6)
C3	N1	C5	C6	-50.0(5)	C7	N1	C3	C4	-

									177.6(5)
C3	N1	C7	C8	-61.4(5)	C7	N1	C5	C6	68.8(5)

Table S7. Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103)

Atom	**X**	**Y**	**Z**	**U(eq)**
H1A	3556.14	3317.22	7284.58	62
H1B	4025.18	4418	7342.67	62
H2A	5693.8	3613.84	8794.85	102
H2B	4220.96	3171.15	9356.88	102
H2C	4577.82	4288.25	9470.13	102
H3A	-138.32	4578.67	6684.5	55
H3B	1499.02	4920.74	6275.45	55
H4A	272.04	3720.06	4986.47	91
H4B	436.96	2987.73	6080.74	91
H4C	1985.22	3388.14	5580.01	91
H5A	1263.29	2736.06	8070.64	52
H5B	1487.72	3285.63	9317.36	52
H6A	-1290.04	3410.36	7619.07	82
H6B	-1065.02	3979.42	8856.44	82
H6C	-1174.84	2841.94	8855.36	82
H7A	556.68	5206.48	8706.76	55
H7B	2173.69	4921.98	9491.98	55
H8A	1972.4	6142.43	7451.25	90
H8B	3597.65	5852.8	8230	90
H8C	2335.15	6492.91	8806.91	90

Table S8. Comparative summary of key photophysical properties of representative lead-free halide scintillators.

Materials	**PLQY (%)**	**Photostability**	**Thermal Decomposition Temperature (℃)**	**Emission Wavelength (nm)**	**Ref.**
$Cs_3Cu_2I_5$	73.7	Stable after 30 days of storage in ambient	--	445	1

		atmosphere			
$Cs_3Cu_2I_5$	60	It retains 60% of its initial PL intensity after 90 days	560	479	2
$Cs_3Cu_2Cl_5$	53	The PL intensity retains 70% of its initial value after 60 days	500	510	2
$[N(C_2H_5)_4]_2Cu_2Br_4$	97.08	Stable after 49 days in ambient atmosphere, 30 h of UV irradiation, and 7 days in pure oxygen	240	463	3
$[PTPP]_2Cu_4I_6$	93.1	Stable after 30 days of storage in ambient atmosphere and 10 hours of UV irradiation.	200	524	4
$(C_8H_{20}N)_2Cu_2Br_4$	99.7	Stable after 2 weeks of storage in ambient atmosphere and 120 minutes of UV irradiation	--	468	5
Rb_2CuCl_3	99.4	Stable after 50 days of storage in ambient atmosphere and 12 hours of UV irradiation	610	397	6
$Cs_3Cu_2I_5$:Mn	54.5	It shows 50% PL intensity retention after 30 days of ambient storage, and 95% retention after 5 thermal cycles	--	445+562	7
$\beta-Cs_3Cu_2Cl_5$	97.3	The PLQY decreases to 41% after 150 days, while the PL intensity remains stable upon 12 hours of UV lamp irradiation	--	526	8
$CsCu_2I_3$	15.7	The PL remains stable within the temperature range of 77–447 K	371	570	9
$(MA)_4Cu2Br_6$	93	Stable after 1 month of storage at 40% relative humidity (RH) and 10 hours of UV irradiation	265	524	10
MA_2CuCl_3	97	After 24 hours of UV irradiation, the PL intensity retains 70%	600	570	11
$(C_4H_9)_4NCuCl_2$	82	Slight degradation after 30 days at 35% RH; 95% PL	260	508	12

	retention after 240 min of UV irradiation	

Figure S1. Preparation of the $TEA_2Cu_2Br_4$ precursor solution by dissolving 2 mmol TEABr and 2 mmol CuBr in 10 mL acetone. The solution was filtered through a 0.45 μm PVDF membrane before crystallization.

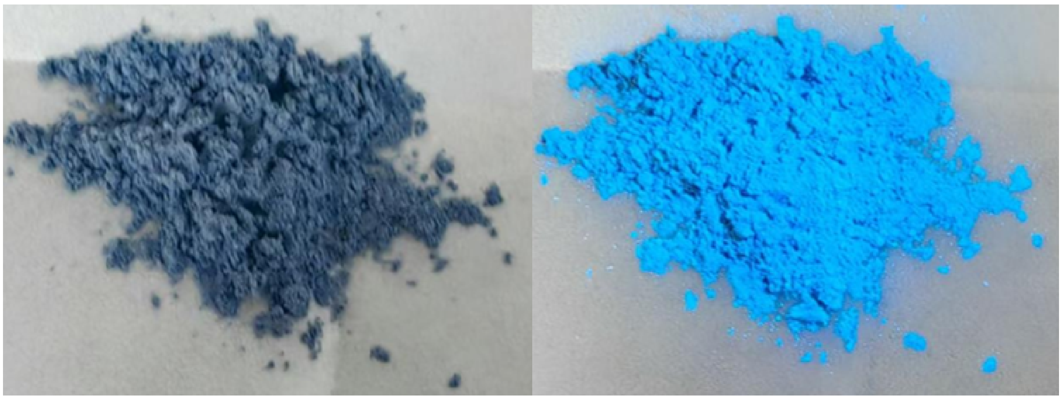

Figure S2. Photographs of $TEA_2Cu_2Br_4$ powder under ambient light and 310 nm UV excitation, showing intense deep-blue emission centered at 478 nm, consistent with the high PLQY (98%) measured for this material.

Figure S3. Transparent millimeter-sized $TEA_2Cu_2Br_4$ single crystals obtained by slow solvent evaporation under ambient conditions (22–25 °C, 45–55% RH) over approximately 48–60 h.

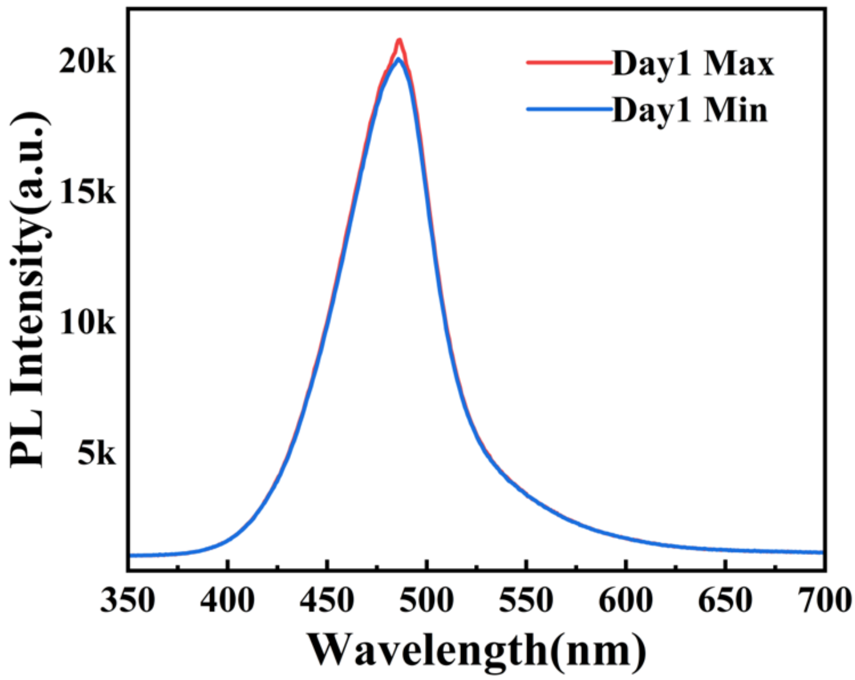

Figure S4. PL Spectrum of $TEA_2Cu_2Br_4$ recorded on the first day of the stability test.

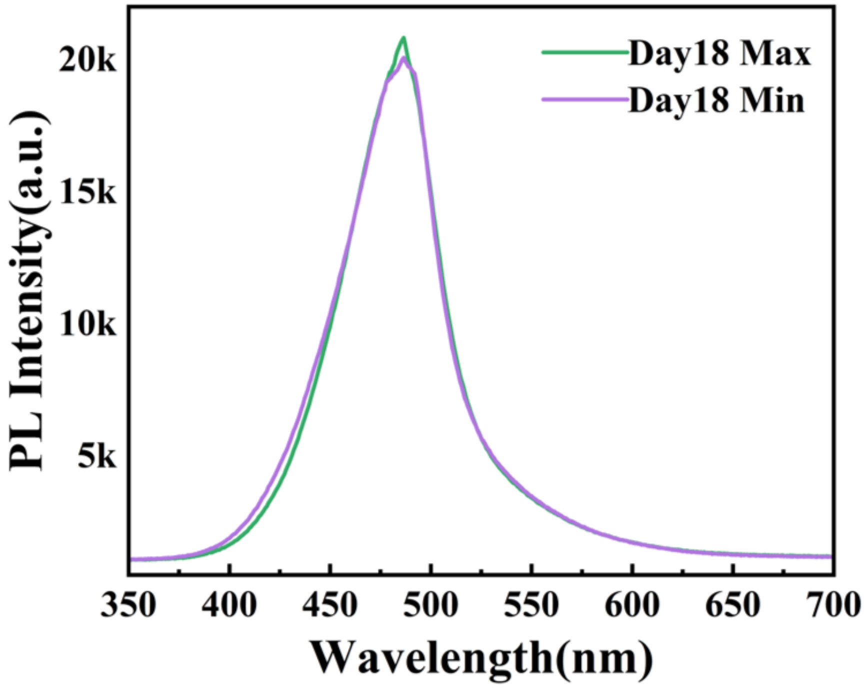

Figure S5. PL Spectrum of $TEA_2Cu_2Br_4$ recorded on the eighteenth day of the stability test.

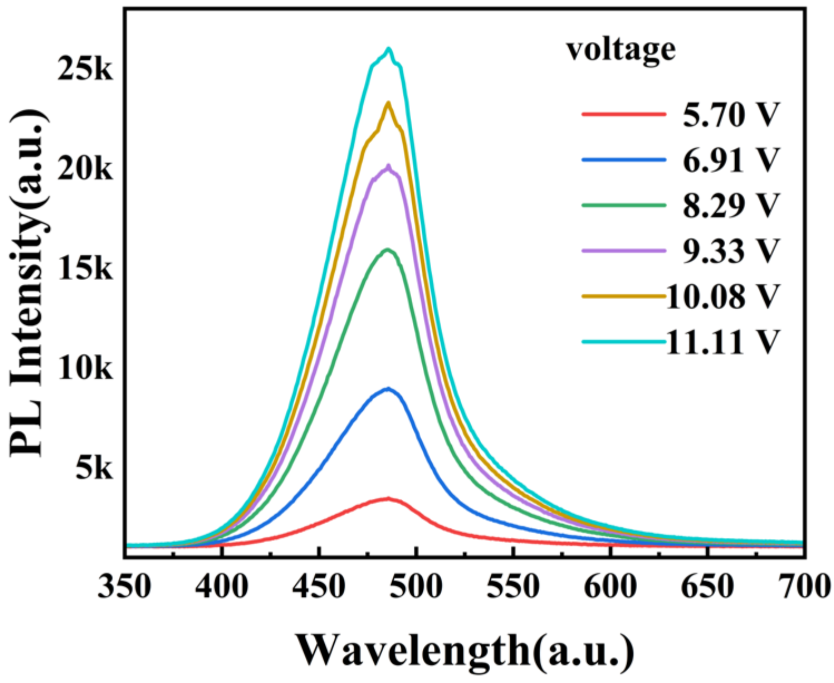

Figure S6. PL Spectrum of $TEA_2Cu_2Br_4$ Under Increasing Voltage.

Figure S7.Stability tests were conducted at 0-50℃.

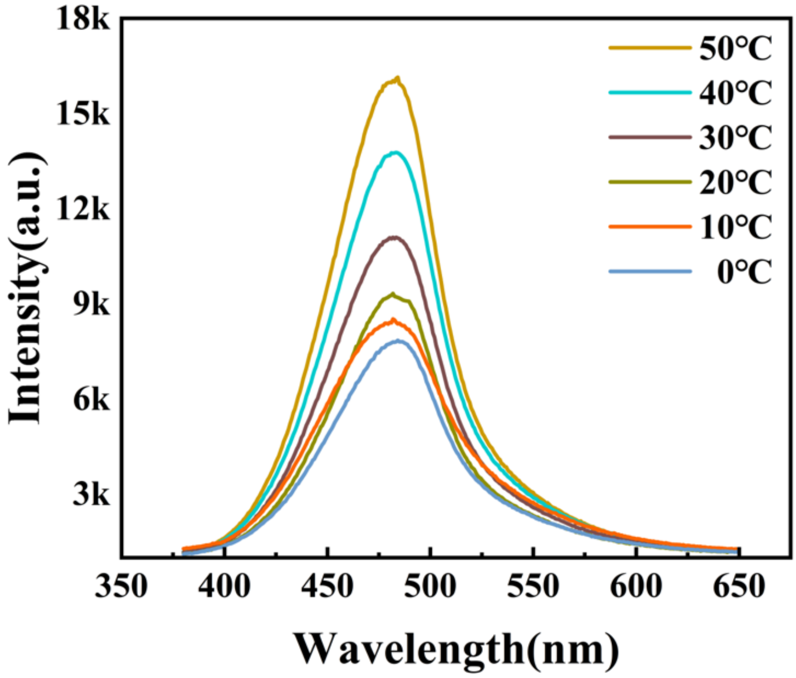

Figure S8. PL Spectrum of $TEA_2Cu_2Br_4$ in the First Cycle of the 50–0℃ Thermal Cycling Test.

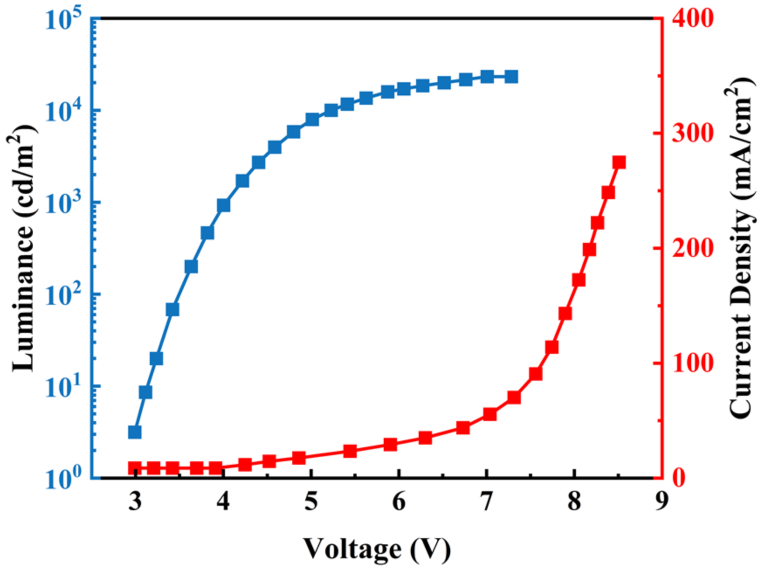

Figure S9. Current density–voltage–luminance (J–V–L) characteristics of the WLED device

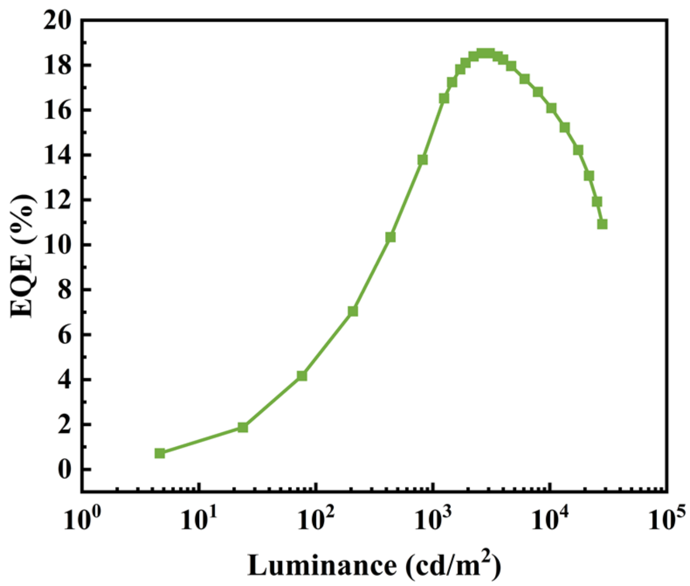

Figure S10. External quantum efficiency (EQE) as a function of luminance for the WLED device.

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