Two Cationic $[(Cu_xI_y)^{x-y}]_n$ Motifs Based Coordination Polymers and Their Photocatalytic Properties

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Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for CPs **1**and **2**.

Table S2. Hydrogen Bonds for CP **2**.

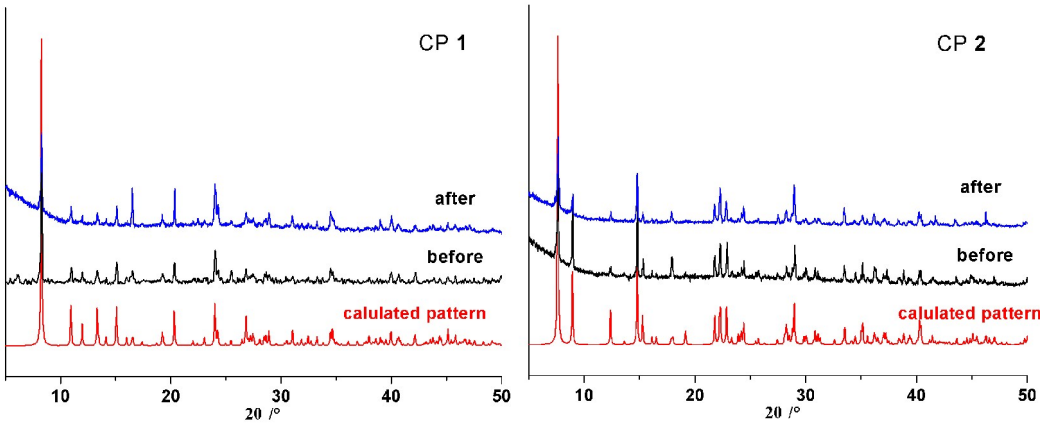

Fig. S1. PXRD comparison of calculated, experimented patterns (before and after successive catalysis for 5 times) of CPs **1** and **2**.

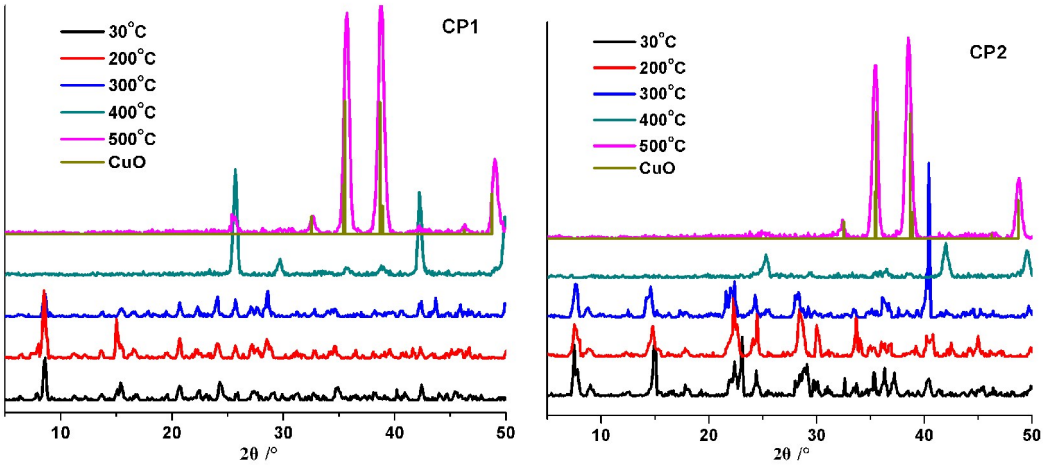

Fig. S2. Variable-temperature XRD of CPs **1** and **2**.

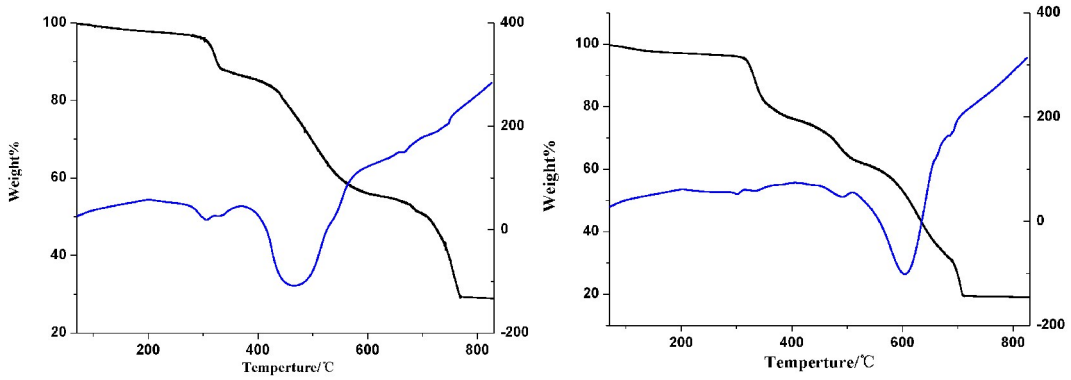

Fig. S3. TGA curves of CPs **1** (left) and **2** (right).

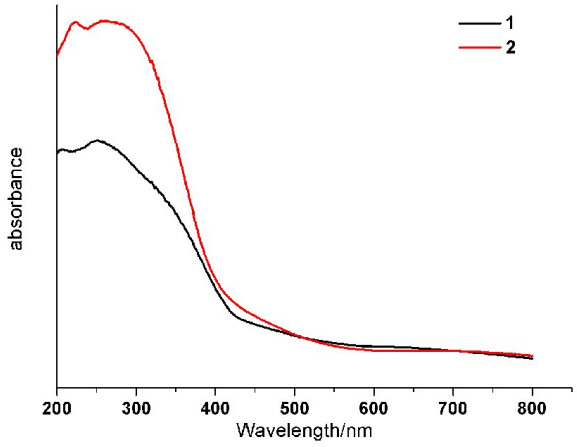

Fig. S4. UV-vis spectra of CPs **1** and **2** in the solid state.

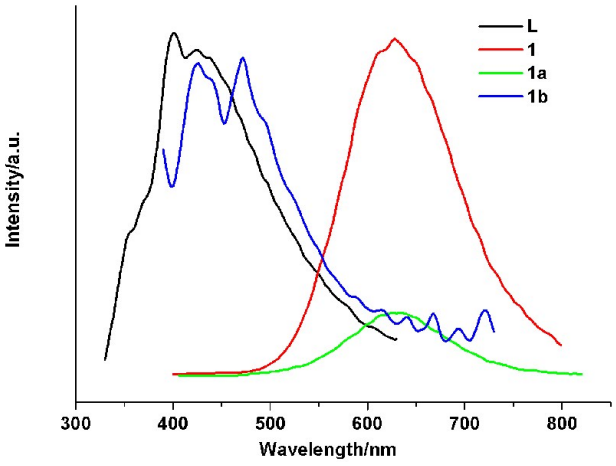

Fig. S5. Luminescent spectra of HTBA, CP **1**, CP **1** at -200 °C and **1a** (CP **1** after treated at 200 °C for 3 h).

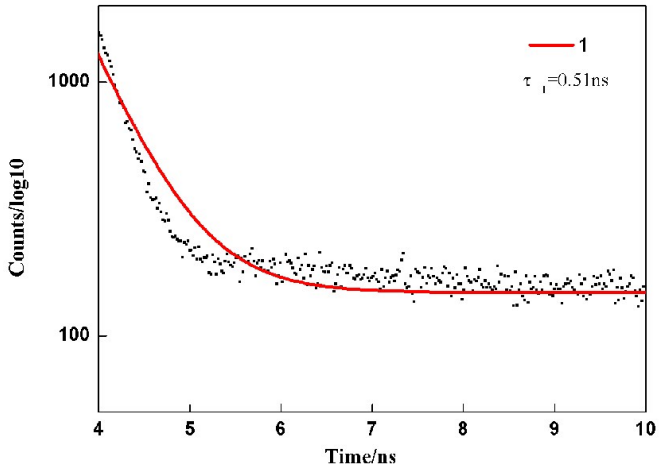

Fig. S6. Lifetime of CP **1**.

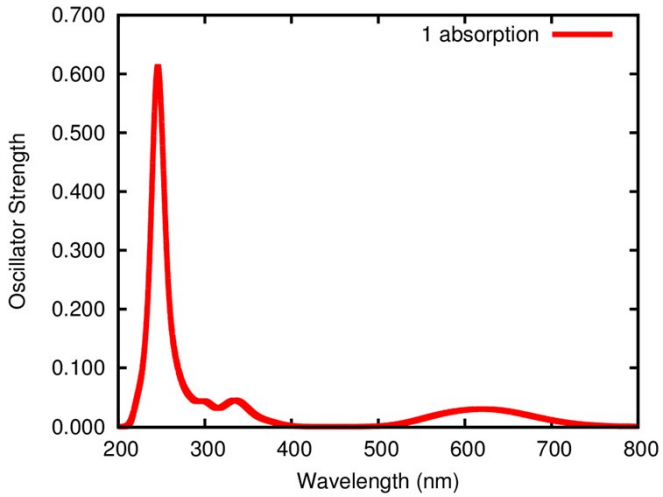

Fig. S7. The simulated excitation spectrum of **1**, TD-M062X/LanL2DZ; 6-31+G(d) level of theory.

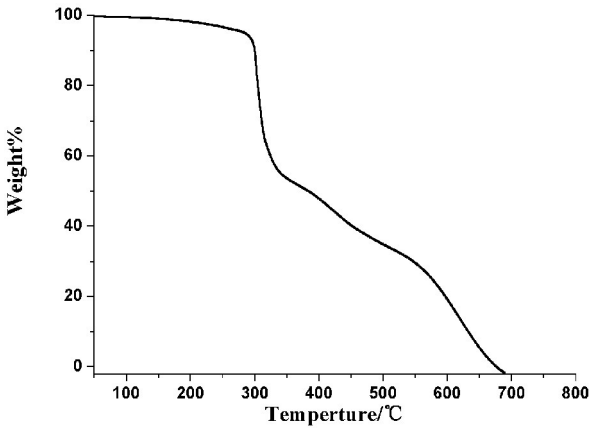

Fig. S8. TGA curve of HTBA.

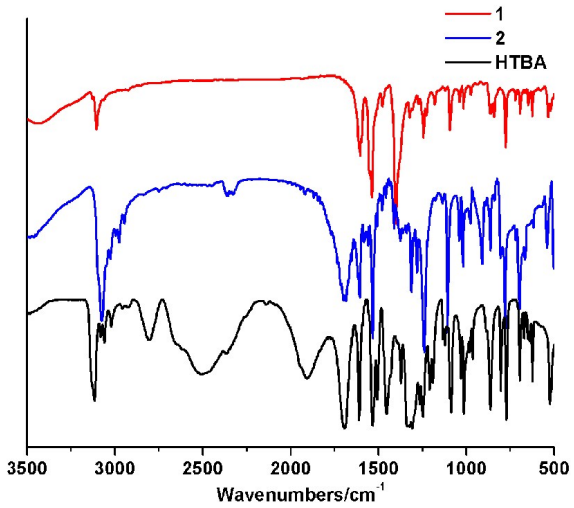

Fig. S9. IR spectra of HTBA, CPs **1** and **2**.

Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for CPs **1** and **2**.

CP **1**			
Bond	Dist.	Bond	Dist.
Cu(1)−N(2)^{I}	2.000(5)	Cu(2)−I(2)	2.6731(10)
Cu(1)−N(3)^{II}	2.015(4)	Cu(2)−I(1)	2.7358(11)

Cu(1)−I(2)	2.6142(9)	Cu(2)−I(1)^{III}	2.7798(12)
Cu(1)−I(1)^{III}	2.7264(10)	Cu(3)−O(1)^{III}	1.933(4)
Cu(2)−O(2)	1.985(4)	Cu(3)−I(2)	2.5376(10)
Cu(2)−Cu(3)	2.4666(12)	Cu(3)−I(1)	2.8191(11)
Angle	(°)	Angle	(°)
N(2)^{I}−Cu(1)−N(3)^{II}	115.67(18)	I(2)−Cu(2)−I(1)	99.61(3)
N(2)^{I}−Cu(1)−I(2)	119.50(15)	O(2)−Cu(2)−I(1)^{III}	107.36(14)
N(3)^{II}−Cu(1)−I(2)	103.76(14)	I(2)−Cu(2)−I(1)^{III}	107.87(4)
N(2)^{I}−Cu(1)−I(1)^{III}	100.88(15)	I(1)−Cu(2)−I(1)^{III}	107.55(4)
N(3)^{II}−Cu(1)−I(1)^{III}	105.07(14)	O(1)^{III}−Cu(3)−I(2)	134.54(14)
I(2)−Cu(1)−I(1)^{III}	111.25(3)	O(1)^{III}−Cu(3)−I(1)	113.32(13)
O(2)−Cu(2)−I(2)	115.91(14)	I(2)−Cu(3)−I(1)	100.82(4)
O(2)−Cu(2)−I(1)	117.90(14)		

Symmetry codes: I: x+1,-y+3/2,z-1/2; II: -x,y-1/2,-z+3/2; III: -x+1, -y+2, -z+1

CP **2**

Bond	Dist.	Bond	Dist.
Cu(1)−N(3)^{I}	1.974(3)	Cu(1)−I(1)^{I}	2.7375(5)
Cu(1)−N(2)	1.983(3)	Cu(1)−I(1)	2.7563(5)
Angle	(°)	Angle	(°)
N(3)^{I}−Cu(1)−N(2)	140.90(13)	N(2)−Cu(1)−I(1)	100.90(9)
N(3)^{I}−Cu(1)−I(1)^{I}	101.12(9)	I(1)^{I}−Cu(1)−I(1)	112.60(2)
N(2)−Cu(1)−I(1)^{I}	101.23(9)	C(2)−N(2)−Cu(1)	126.6(2)
N(3)^{I}−Cu(1)−I(1)	99.53(9)	N(3)−N(2)−Cu(1)	124.0(2)

Symmetry codes: I: x,-y+1,z-1/2

Table S2. Hydrogen Bonds for CP **2**

D−H...A	d(D−H)	d(H...A)	d(D...A)
O(2)−H(2A)···O(2)$^{\#5}$	0.82	1.70	2.473(5)
O(3)−H(31)···O(1)$^{\#6}$	0.85	2.30	2.962(11)
O(3)−H(32)···O(1)$^{\#7}$	0.85	2.09	2.844(12)

Symmetry codes: 5: -x+1/2,-y-1/2,-z;6: x,-y,z+1/2; 7: -x+1,-y,-z+1