Supporting Information

A novel 3-D cuprous iodide polymer with a high Cu/I ratio

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General Remarks. All analytical grade chemicals were obtained commercially and used without further purification. Elemental analyses (C, N and H) were performed using a PE2400 II elemental analyzer. IR spectra were obtained from a powdered sample pelletized with KBr on an ABB Bomen MB 102 series IR spectrophotometer in the range of 400–4000cm^{-1}. PXRD patterns were obtained using a Bruker D8 Advance XRD diffractometer with Cu Kα radiation (λ = 1.54056 Å). The photoluminescence spectra were recorded at room temperature with a modular double grating excitation spectrofluorimeter with a TRIAX 320 emission monochromator (Fluorolog-3, Horiba Scientific) coupled to an R928 Hamamatsu photomultiplier. The excitation source was a 450 W Xe arc lamp. The emission spectra were corrected for detection and optical spectral response of the spectrofluorimeter and the excitation spectra were corrected for the spectral distribution of the lamp intensity using a photodiode reference detector.

Crystal Structure Determinations

The intensity data were collected on a Rigaku Mercury CCD diffractometer with graphite monochrochromated Mo Kα radiation (λ = 0.71073Å) at 100-293K. The absorption corrections were applied using multi-scan technique. The structures were solved by direct methods using SHELXS-97 and refined by full-matrix least-squares on F^2 using the SHELXL-97 program. The non-hydrogen atoms were refined anisotropically. H atoms were placed in idealized locations and refined as riding. Technical details of data collections and refinement are summarized in Table S1.

Table S1 Crystallographic data for **1** at multi-temperature.

formula	$C_8H_4Cu_3IN_8$	$C_8H_4Cu_3IN_8$	$C_8H_4Cu_3IN_8$	$C_8H_4Cu_3IN_8$
Fw	529.74	529.74	529.74	529.74
crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	C2/m	C2/m	C2/m	C2/m
a, Å	13.790(5)	13.766(2)	13.716(2)	13.696(3)
b, Å	12.700(3)	12.7157(18)	12.690(2)	12.695(2)
c, Å	8.1008(18)	8.0750(11)	8.0424(14)	8.0211(14)
β, deg	125.962(3)	125.800(2)	125.674(2)	125.512(2)
V, Å^3	1148.3(5)	1146.5(3)	1137.1(3)	1135.3(4)
Z	4	4	4	4
T, K	293(2)	220(2)	180(2)	100(2)
Calcd density,Mg.m^{-3}	3.064	3.069	3.094	3.100
abs coeff, mm^{-1}	8.193	8.207	8.273	8.288
F(*000*)	992	992	992	992
2*θ*(max), deg	50.20	50.20	50.18	50.20
Total reflns collected	4107	4030	3509	4019
Unique reflns	1067	1056	1043	1050
No. of param	98	98	98	98
*R*1[*I*>2σ(*I*)]	0.0206	0.0194	0.0188	0.0181
*wR*2(all data)	0.0542	0.0498	0.0548	0.0452
GOF on F^2	1.078	1.093	1.157	1.148

Table S2 Selected bond lengths [Å] of **1** at different temperature.

	293 K	220 K	180 K	100 K
Cu-I	2.7348(6)- 3.0736(8)	2.7273(5)- 3.0726(6)	2.7159(5)- 3.0652(6)	2.7085(5)- 3.0640(6)
Cu-N	1.906(3)-2.010(3)	1.907(3)- 2.011(3)	1.902(3)-2.007(3)	1.904(3)-2.005(3)
Cu1#1···Cu3	3.387	3.396	3.395	3.402
Cu2···Cu2#2	3.370	3.362	3.348	3.337

Symmetry transformations used to generate equivalent atoms: (#1) -x+1,-y,-z+1; (#2) -x+1,-y,-z.

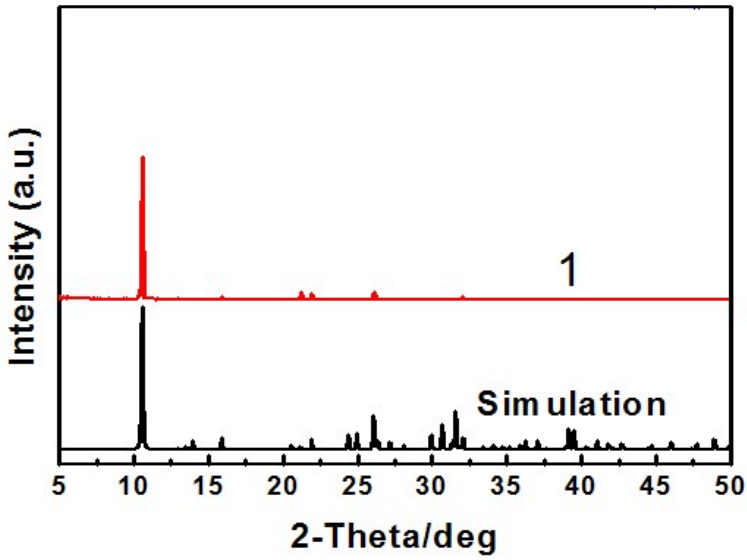


Fig. S1 Simulated and experimental powder XRD patterns of **1**.

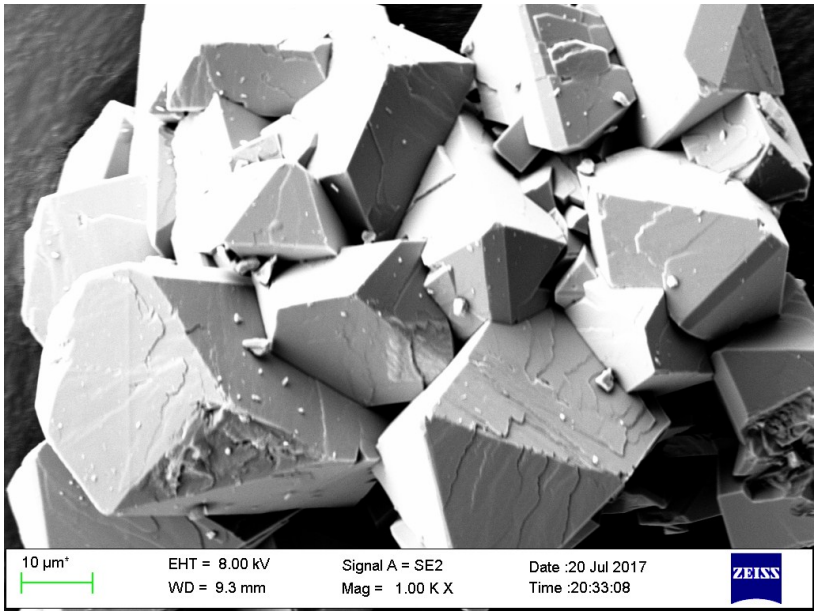


Fig. S2 SEM of **1**.

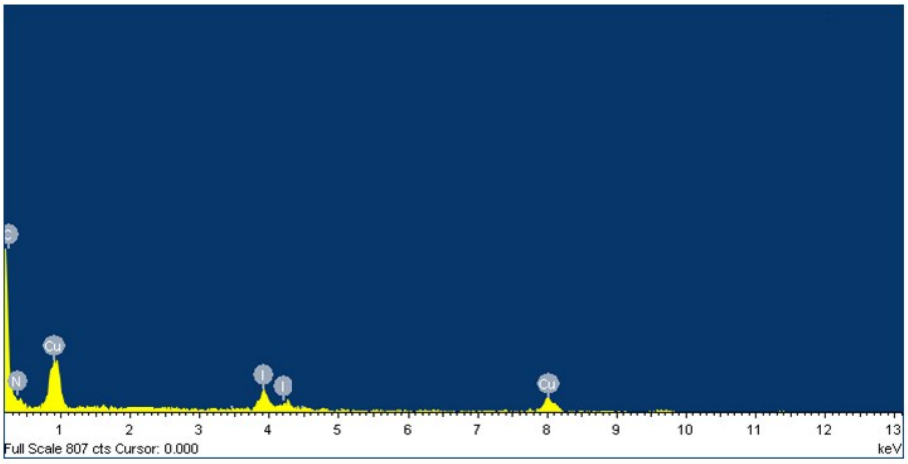


Fig. S3. EDS spectrum of **1**.

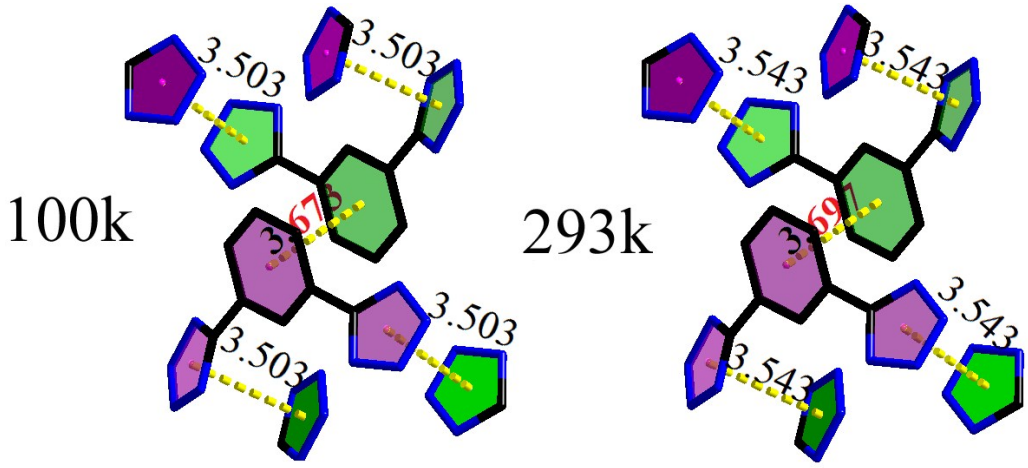


Fig. S4. The strong π···π stacking interactions between neighbor phenyl rings or tetrazolate rings.

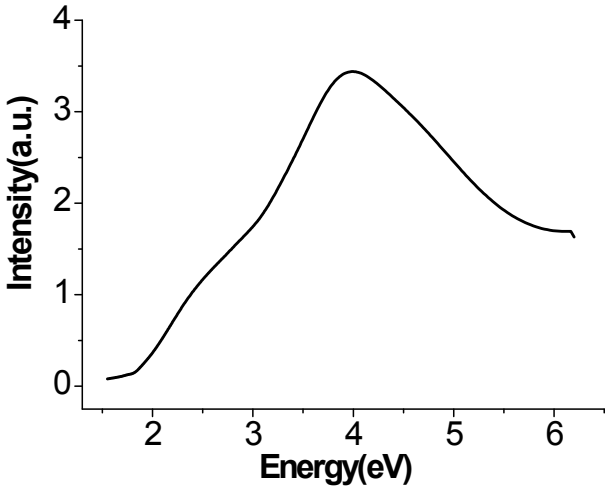


Figure S5 Optical diffuse reflection spectrum of **1**.

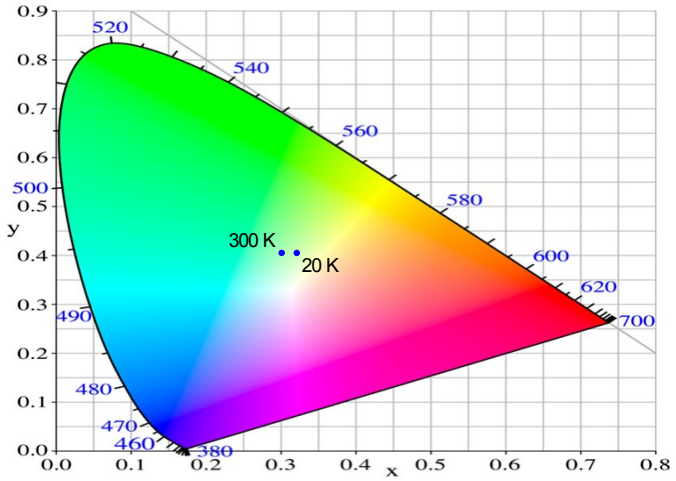


Fig. S6. CIE chromaticity diagram for **1** at 20 K and 40 K (λ_{ex} = 340 nm).

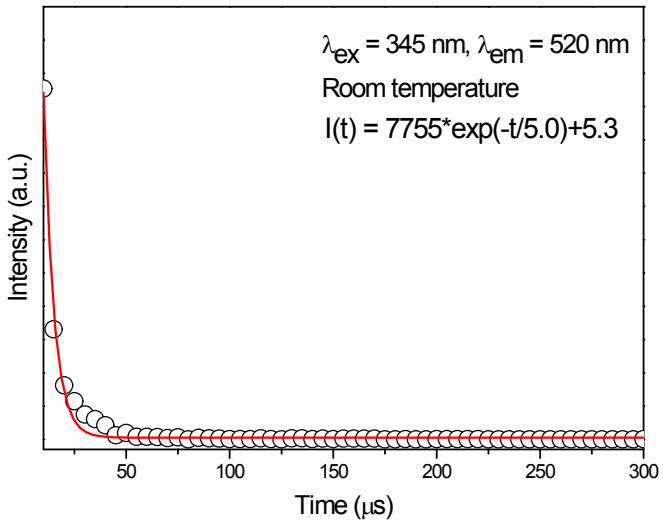
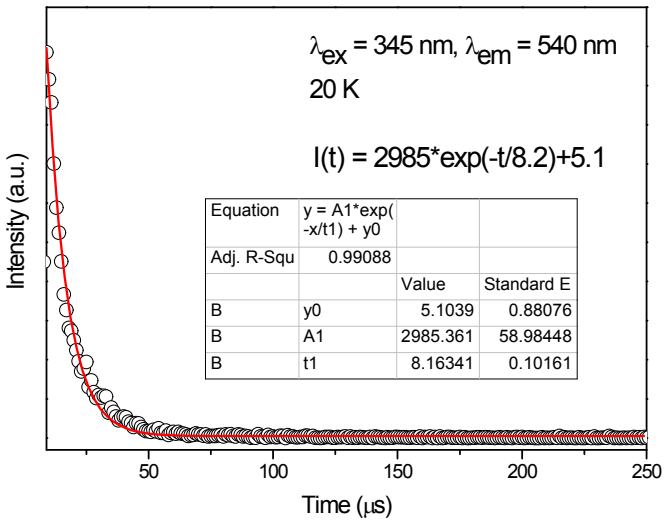


Fig. S7. Decay curve of **1** at room temperature (λ_{ex} = 345 nm, λ_{em} = 520 nm).



Equation	y = A1*exp(-x/t1) + y0		
Adj. R-Squ	0.99088		
		Value	Standard E
B	y0	5.1039	0.88076
B	A1	2985.361	58.98448
B	t1	8.16341	0.10161

Fig. S8 Decay curve of **1** at 20 K (λ_{ex} = 345 nm, λ_{em} = 540 nm).

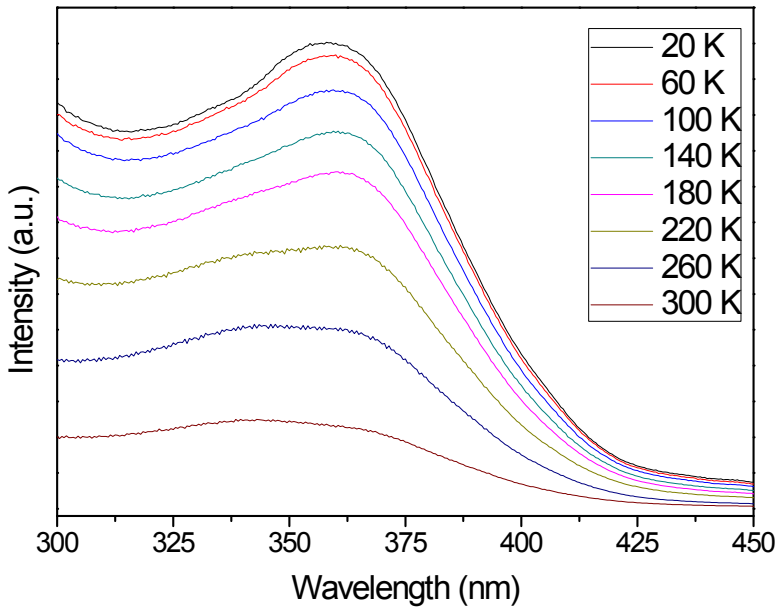


Fig. S9. Excitation spectra of **1** at different temperatures.

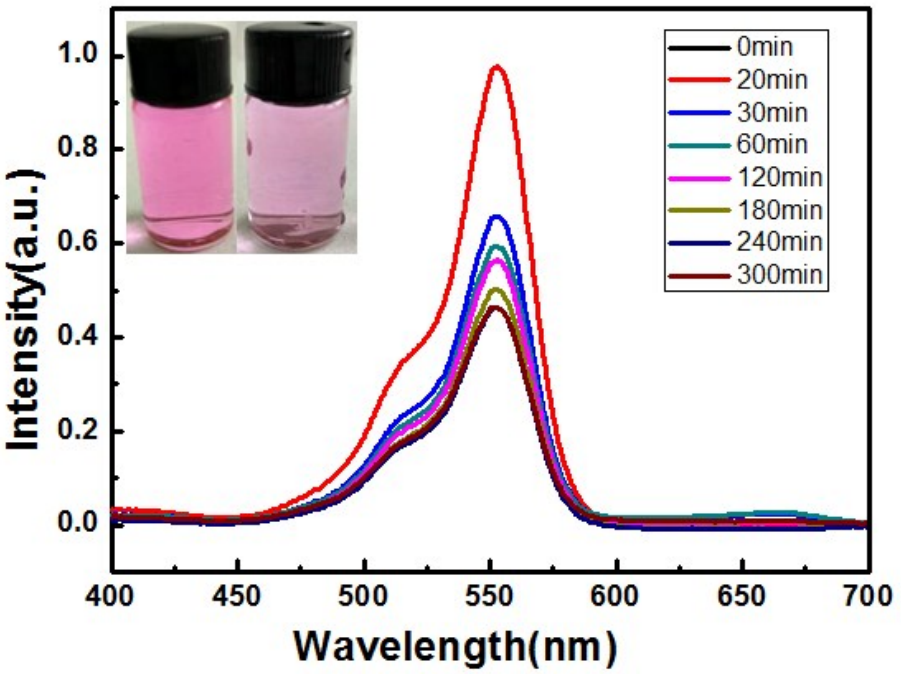


Fig. S10 UV-vis absorption spectra for degradation of RhB by using **1** as photocatalyst.

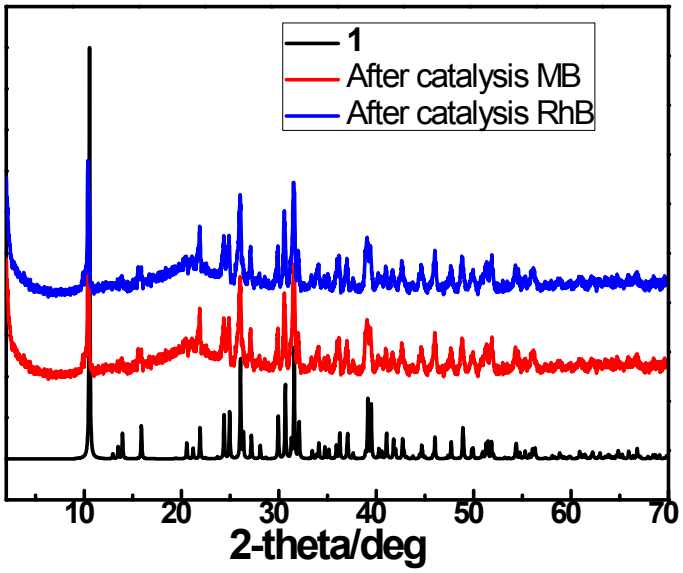


Fig. S11 Experimental and after catalysis of MB or RhB powder XRD patterns of **1**.