Electronic Supplementary Information

Assembly of Zn^{II}-coordination polymers constructed by benzothiadiazole functionalized bipyridines and V-shaped dicarboxylic acids: topology variety, photochemical and visible-light-driven photocatalytic properties

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Table S1 Selected bond lengths (Å) and angles (°) for complexes **1**–**4**[a]

		1	
Zn(1)-O(1)	1.987(4)	Zn(1)-N(4)	2.048(5)
Zn(1)-O(2)$^{\#2}$	2.076(4)	Zn(1)-O(1)$^{\#3}$	1.987(4)
Zn(1)-O(2)$^{\#1}$	2.076(4)		
O(1)$^{\#3}$-Zn(1)-O(2)$^{\#2}$	90.00(15)	O(1)$^{\#3}$-Zn(1)-N(4)	101.75(12)
O(1)-Zn(1)-O(2)$^{\#2}$	86.81(15)	O(2)$^{\#1}$-Zn(1)-N(4)	97.84(12)
O(1)-Zn(1)-N(4)	101.75(12)	O(2)$^{\#1}$-Zn(1)-O(2)$^{\#2}$	164.3(2)
O(2)$^{\#2}$-Zn(1)-N(4)	97.84(12)	O(1)$^{\#3}$-Zn(1)-O(2)$^{\#1}$	86.81(15)
O(1)-Zn(1)-O(2)$^{\#1}$	90.01(15)	O(1)-Zn(1)-O(1)$^{\#3}$	156.5(2)
		2	
Zn(1)-O(9)$^{\#1}$	2.355(4)	Zn(1)-N(1)	2.024(4)
Zn(1)-O(1)	1.956(3)	Zn(1)-O(10)$^{\#1}$	2.000(4)
Zn(1)-O(6)	1.988(3)	Zn(2)-O(2)	2.006(3)
Zn(2)-O(4)$^{\#2}$	2.008(4)	Zn(2)-O(5)$^{\#2}$	2.332(4)
Zn(2)-O(7)	1.964(4)	Zn(2)-N(4)$^{\#3}$	2.051(4)
O(1)-Zn(1)-O(6)	101.30(16)	O(5)$^{\#2}$-Zn(2)-N(4)$^{\#3}$	91.94(15)
O(1)-Zn(1)-O(9)$^{\#1}$	88.97(15)	O(1)-Zn(1)-O(10)$^{\#1}$	132.29(16)
O(6)-Zn(1)-O(9)$^{\#1}$	161.00(14)	O(6)-Zn(1)-O(10)$^{\#1}$	102.05(15)
O(9)$^{\#1}$-Zn(1)-O(10)$^{\#1}$	59.83(14)	O(5)$^{\#2}$-Zn(2)-O(2)	159.84(14)
O(2)-Zn(2)-N(4)$^{\#3}$	98.12(16)	O(4)$^{\#2}$-Zn(2)-O(2)	100.44(15)
O(4)$^{\#2}$-Zn(2)-O(5)$^{\#2}$	60.14(14)	O(2)-Zn(2)-O(7)	102.60(15)
O(4)$^{\#2}$-Zn(2)-O(7)	142.52(16)	O(5)$^{\#2}$-Zn(2)-O(7)	91.99(14)
O(4)$^{\#2}$-Zn(2)-N(4)$^{\#3}$	102.47(16)	N(4)$^{\#3}$-Zn(2)-O(7)	103.05(16)
O(1)-Zn(1)-N(1)	104.84(16)	N(1)-Zn(1)-O(6)	100.11(15)
O(9)$^{\#1}$-Zn(1)-N(1)	92.50(15)	O(10)$^{\#1}$-Zn(1)-N(1)	111.15(16)
		3	
Zn(1)-O(1)	1.965(3)	Zn(1)-N(1)	2.049(4)
Zn(1)-O(9)$^{\#1}$	2.014(4)	Zn(1)-O(10)$^{\#1}$	2.311(5)
Zn(1)-O(6)	1.997(4)	Zn(2)-N(5)	2.021(4)
Zn(2)-O(4)$^{\#2}$	2.464(4)	Zn(2)-O(5)$^{\#2}$	1.962(4)
Zn(2)-O(7)	1.950(4)	Zn(2)-O(2)	1.981(3)
O(1)-Zn(1)-O(6)	100.74(17)	O(1)-Zn(1)-N(1)	98.96(17)
O(1)-Zn(1)-O(9)$^{\#1}$	145.28(17)	O(1)-Zn(1)-O(10)$^{\#1}$	95.80(15)
O(6)-Zn(1)-O(9)$^{\#1}$	96.78(17)	O(6)-Zn(1)-O(10)$^{\#1}$	155.03(16)
O(6)-Zn(1)-N(1)	103.24(18)	O(9)$^{\#1}$-Zn(1)-O(10)$^{\#1}$	59.82(16)
O(9)$^{\#1}$-Zn(1)-N(1)	105.90(18)	O(10)$^{\#1}$-Zn(1)-N(1)	92.42(17)
O(4)$^{\#2}$-Zn(2)-O(2)	163.06(15)	O(2)-Zn(2)-N(5)	98.84(15)
O(5)$^{\#2}$-Zn(2)-O(2)	105.38(15)	O(4)$^{\#2}$-Zn(2)-O(5)$^{\#2}$	58.15(15)
O(5)$^{\#2}$-Zn(2)-N(5)	113.99(16)	O(2)-Zn(2)-O(7)	103.46(16)
O(4)$^{\#2}$-Zn(2)-O(7)	85.04(16)	O(5)$^{\#2}$-Zn(2)-O(7)	123.98(17)
O(7)-Zn(2)-N(5)	107.56(17)	N(5)-Zn(2)-O(4)$^{\#2}$	92.34(15)

4			
Zn(1)-O(1)	2.035(3)	Zn(1)-N(1)	2.029(4)
Zn(1)-O(6)$^{\#1}$	2.039(3)	Zn(1)-O(1)$^{\#2}$	2.035(3)
Zn(1)-O(6)$^{\#3}$	2.039(3)	Zn(2)-O(2)$^{\#3}$	2.058(2)
Zn(2)-N(4)$^{\#6}$	2.015(4)	Zn(2)-O(2)$^{\#4}$	2.058(2)
Zn(2)-O(5)	2.052(3)	Zn(2)-O(5)$^{\#5}$	2.052(3)
O(1)-Zn(1)-N(1)	97.72(8)	N(1)-Zn(1)-O(6)$^{\#3}$	104.70(8)
O(1)$^{\#2}$-Zn(1)-O(6)$^{\#3}$	89.73(13)	O(2)$^{\#3}$-Zn(2)-O(5)	86.30(12)
O(1)-Zn(1)-O(6)$^{\#3}$	86.36(13)	O(2)$^{\#4}$-Zn(2)-N(4)$^{\#6}$	104.48(7)
O(2)$^{\#4}$-Zn(2)-O(5)	89.97(12)	O(5)-Zn(2)-N(4)$^{\#6}$	97.47(8)
O(1)$^{\#2}$-Zn(1)-O(1)	164.55(16)	O(1)$^{\#2}$-Zn(1)-O(6)$^{\#1}$	86.36(13)
O(1)-Zn(1)-O(6)$^{\#1}$	89.73(13)	O(6)$^{\#3}$-Zn(1)-O(6)$^{\#1}$	150.60(16)
O(1)$^{\#2}$-Zn(1)-N(1)	97.72(8)	N(1)-Zn(1)-O(6)$^{\#1}$	104.70(8)
O(2)$^{\#4}$-Zn(2)-O(2)$^{\#3}$	151.04(15)	O(5)$^{\#5}$-Zn(2)-O(2)$^{\#4}$	86.30(12)
O(5)-Zn(2)-O(5)$^{\#5}$	165.07(15)	O(5)-Zn(2)-O(2)$^{\#3}$	89.97(12)
O(2)$^{\#3}$-Zn(2)-N(4)$^{\#6}$	104.48(8)	O(5)$^{\#5}$-Zn(2)-N(4)$^{\#6}$	97.47(8)

[a]Symmetry codes for **1**: $^{\#1}$ 2 – *x*, 1 – *y*, *z* ; $^{\#2}$ 3/2 – *x*, 3/2 – y, 3/2 – z; $^{\#3}$ *x* – 1/2, *y* + 1/2, 3/2 – z; $^{\#4}$ 3/2 – x, *y*, 3/4 – z; $^{\#5}$ 1 – *x*, – *y*, *z*; $^{\#6}$1/2 – *x*, 1/2 – y, 3/2 – z. Symmetry codes for **2**: $^{\#1}$ *x* – 1/2, *y* + 1/2, z; $^{\#2}$ *x* + 1/2, *y* + 1/2, z; $^{\#3}$ 1 + *x*, 1 – *y*, 3/2 + z; $^{\#4}$ *x* – 1/2, *y* – 1/2, z; $^{\#5}$ *x* + 1/2, *y* – 1/2, z; $^{\#6}$ –1 + *x*, 1 – *y*, – 3/2 + z. Symmetry codes for **3**: $^{\#1}$ *x*, – 1 + y, *z*; $^{\#2}$ – 1 + *x*, – 1 + y, *z*; $^{\#3}$ 1 + *x*, 1 + *y*, *z*; $^{\#4}$ *x*, 1 + *y*, *z*; $^{\#5}$ –1 – *x*, – *y*, –1 – *z*. Symmetry codes for **4**: $^{\#1}$ 1 + *x*, *y*, *z*; $^{\#2}$ 5/2 – *x*, *y*, 1 – *z*; $^{\#3}$ 3/2 – *x*, *y*, 1 – *z*; $^{\#4}$ –1 + *x*, *y*, *z*; $^{\#5}$ 1/2 – *x*, *y*, 1 – *z*; $^{\#6}$ –1 + *x*, 1 + *y*, *z*; $^{\#7}$ 1 + *x*, –1 + *y*, *z*.

Table S2 The details data of K_{obs} for the degradation of organic dye.

Complex	K_{obs} (min^{-1}) for RhB	K_{obs} (min^{-1}) for MB	K_{obs} (min^{-1}) for CV
1	0.0024	0.0028	0.0024
2	0.0184	0.0065	0.0044
3	0.0104	0.0034	0.0013
4	0.0073	0.0036	0.0026

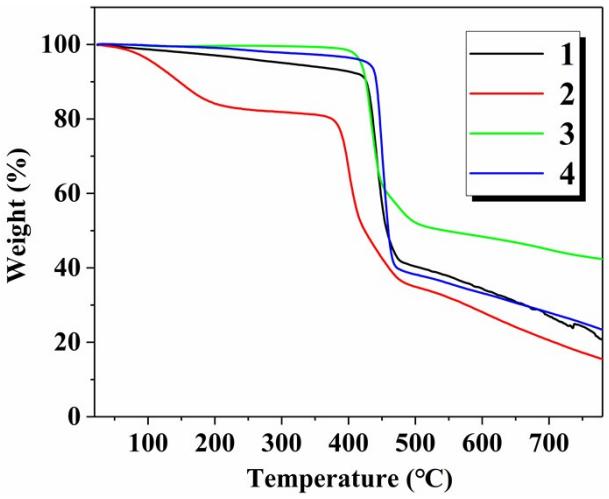


Fig. S1 TGA curves of complexes **1**–**4**.

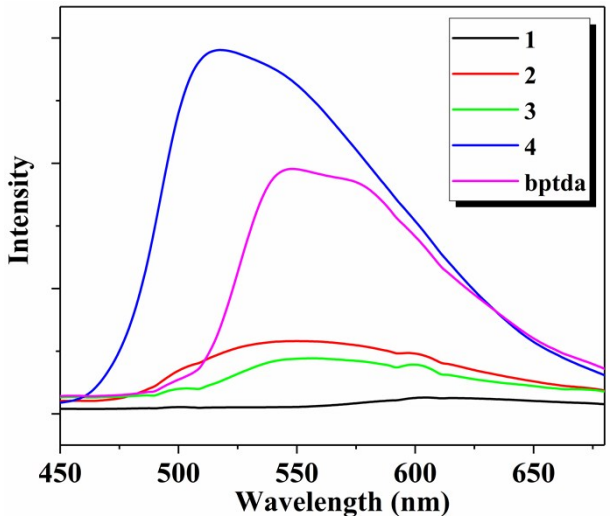
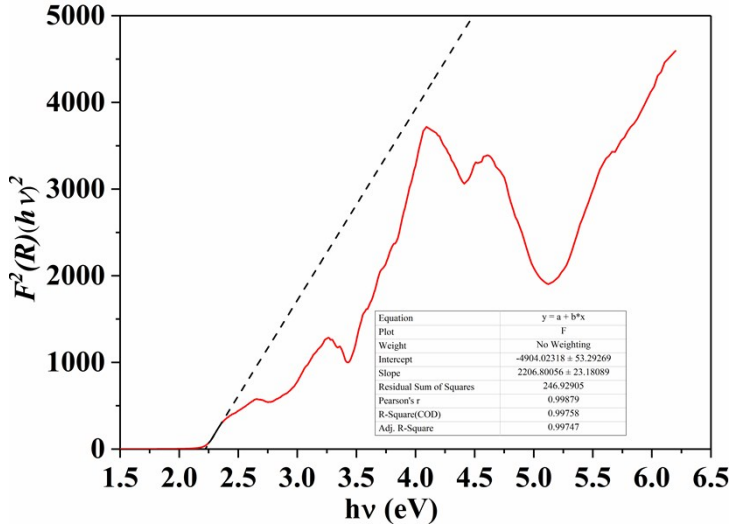
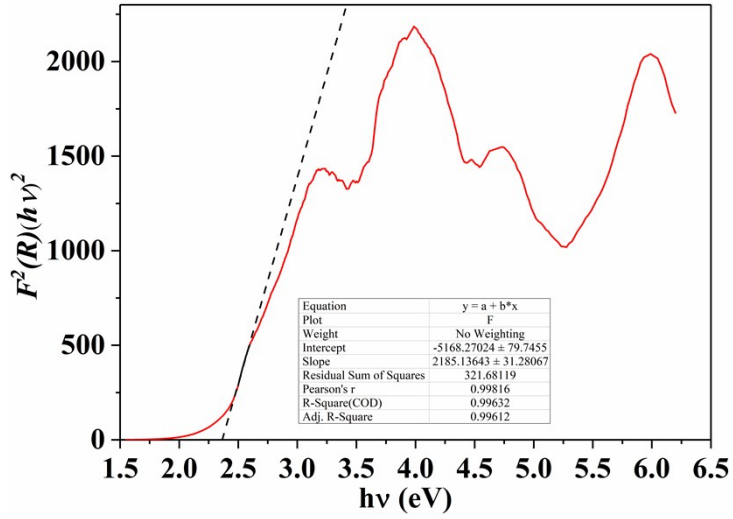


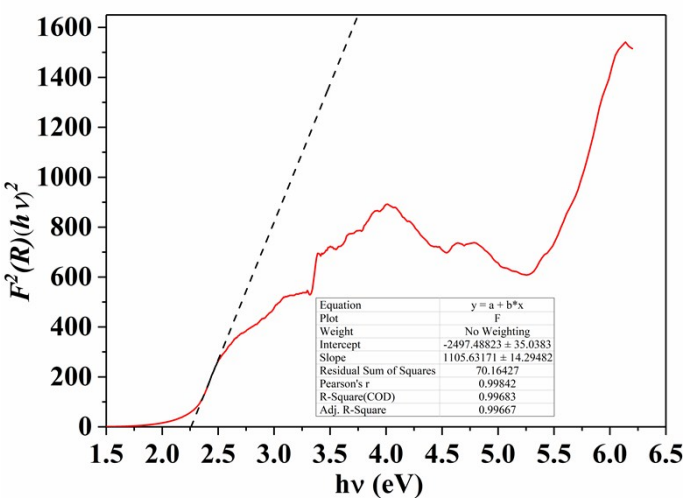
Fig. S2 Fluorescence spectra of complexes **1**–**4** and the bptda ligand.



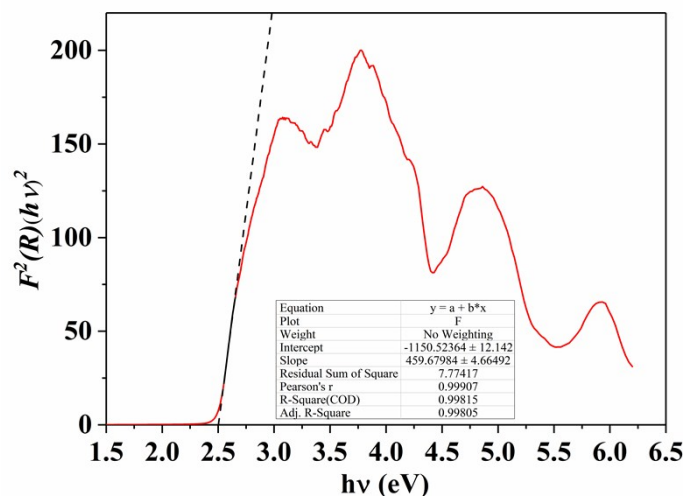
(a)



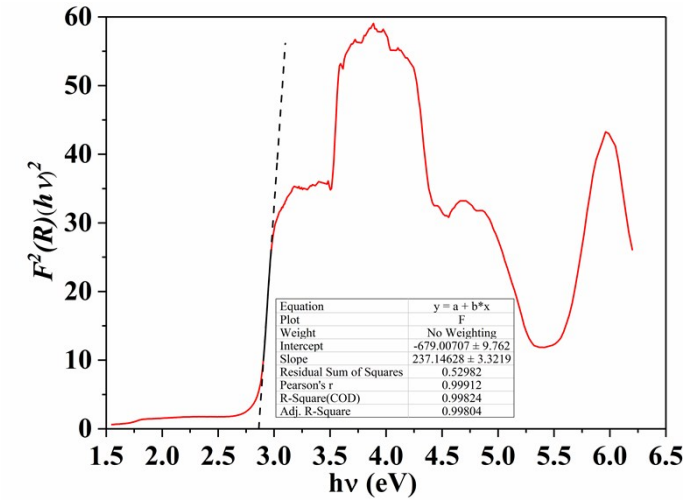
(b)



(c)



(d)



(e)

Fig. S3 Tauc plots for complexes **1** (a), **2** (b), **3**, (c), **4** (d) and **4c** (e) at room temperature, the dashed lines represent fits of the linear regions.

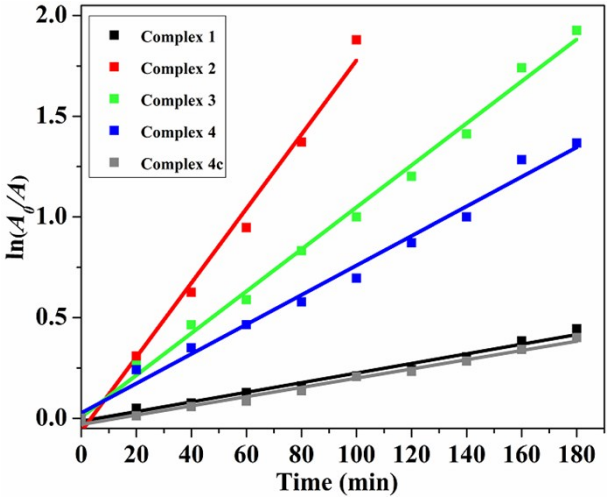
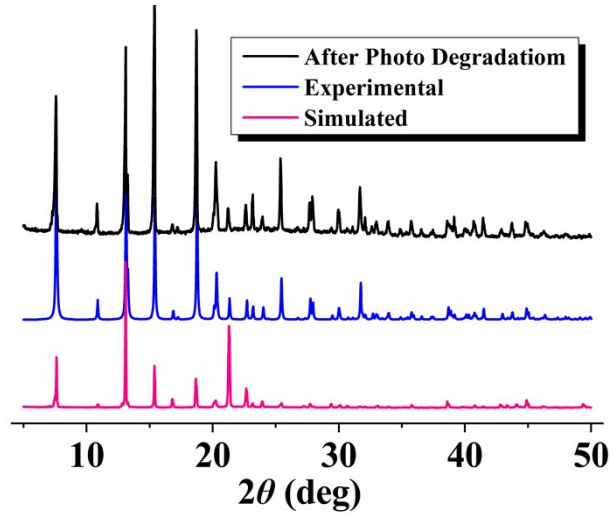
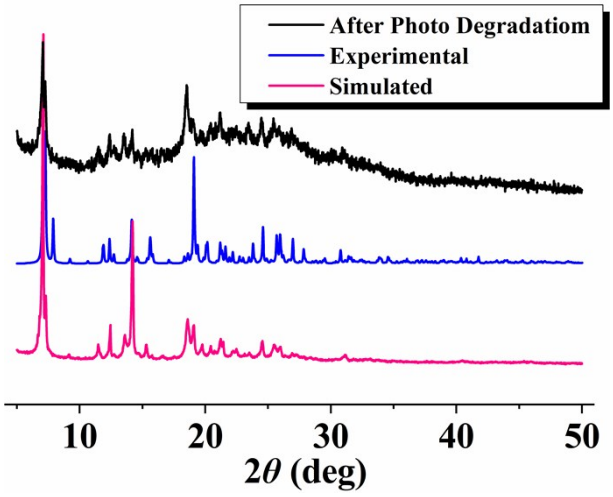


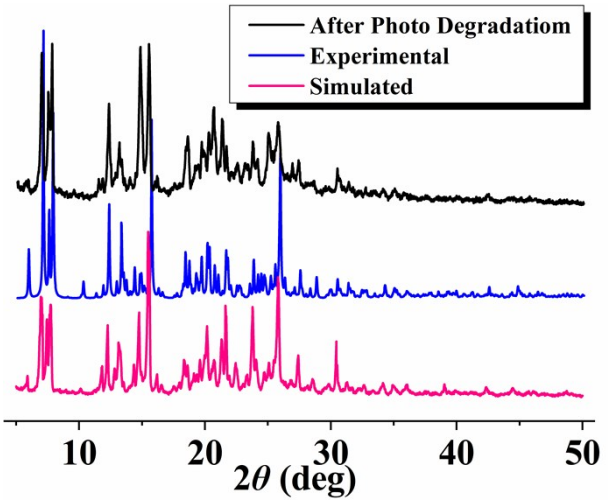
Fig. S4 The plot of ln(A_0/A) versus time.



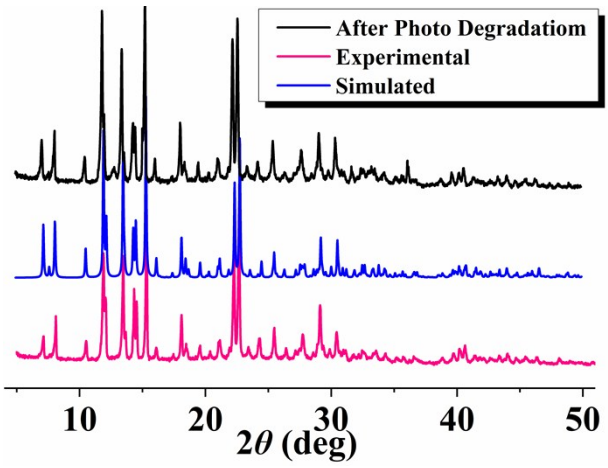
(a)



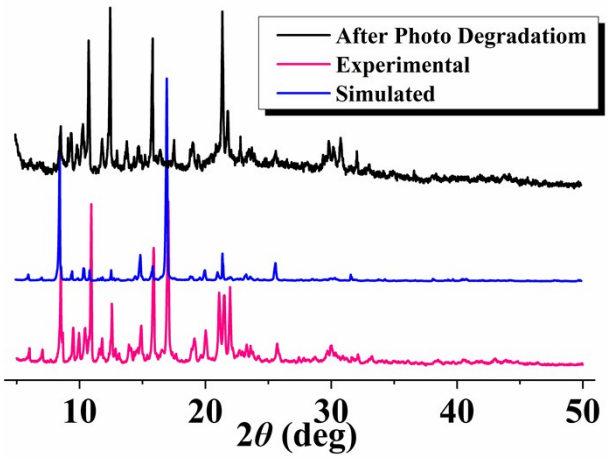
(b)



(c)



(d)



(e)

Fig. S5 PXRD patterns of complexes **1** (a), **2** (b), **3**, (c), **4** (d) and **4c** (e) before and after photo degradation.

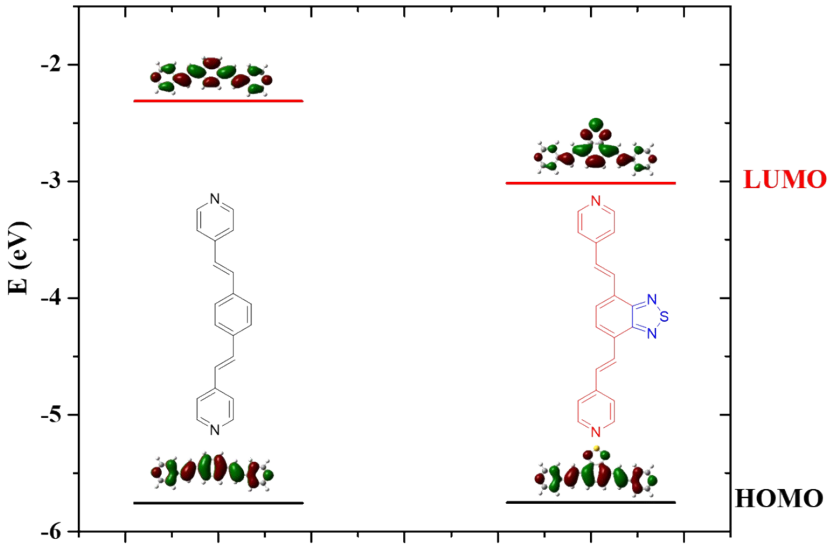


Fig. S6 HOMO and LUMO of the ligands.

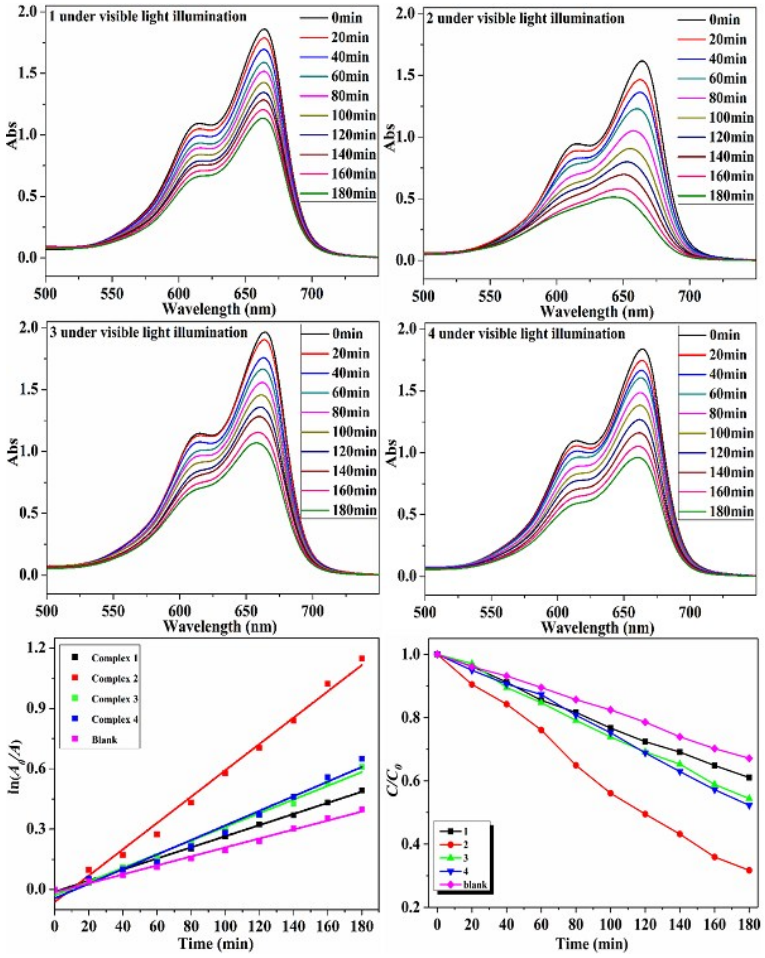


Fig. S7 UV-visible spectral changes of MB aqueous solution, the plot of ln(A_0/A) versus time, and the degradation curve during the photocatalytic degradation reactions in presence of the complexes **1**–**4**; the purple curve is the control experiment without any catalyst.

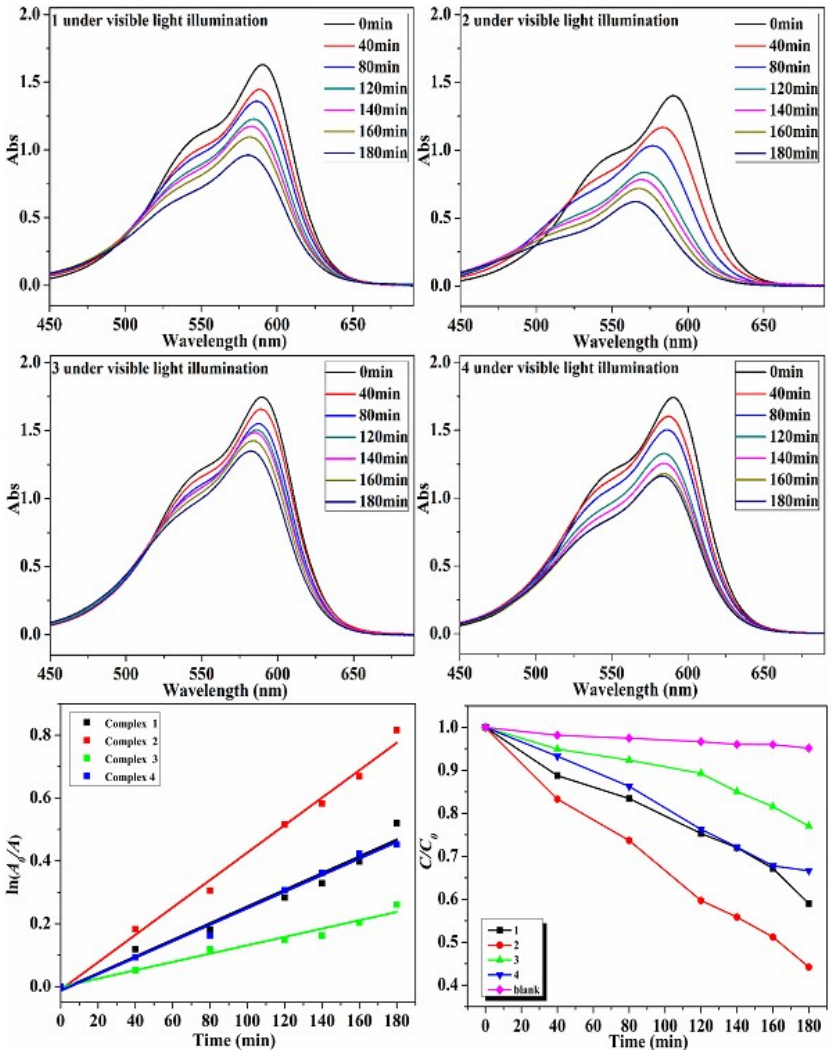


Fig. S8 UV-visible spectral changes of CV aqueous solution, the plot of ln(A_0/A) versus time, and the degradation curve during the photocatalytic degradation reactions in presence of the complexes **1**–**4**; the purple curve is the control experiment without any catalyst.

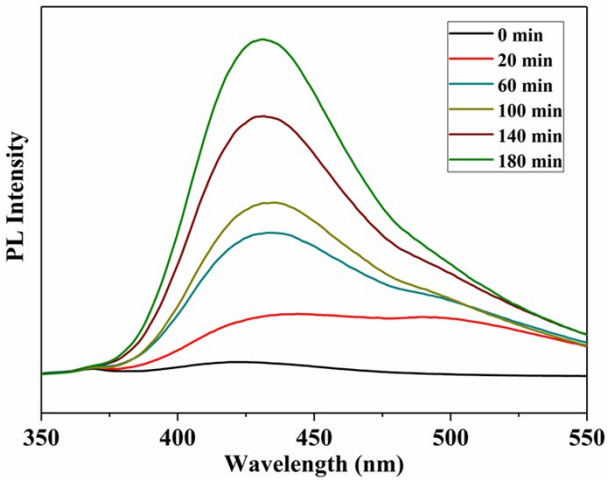


Fig. S9 Photoluminescence spectral changes of the basic solution of terephthalic acid with light irradiation time on complex 4 (excitation at 325 nm)