Electronic supplementary information (ESI)

Alkyl groups-directed assembly of coordination polymers based on bis-(4-imidazol-1-yl-phenyl)-amine and their photocatalytic properties

Hong-Jian Cheng*, Ya-Li Shen, Yi-Feng Lu, Ji Ma, Hong-Wei Ji, Wen-Yu Yin, Xiao-Yan Tang, Yun-Sheng Ma and Rong-Xin Yuan*

School of Chemistry and Materials Engineering, Jiangsu Key Laboratory of Advanced Functional Materials, Changshu Insititute of Technology, Changshu, Jiangsu, 215500, P. R. China

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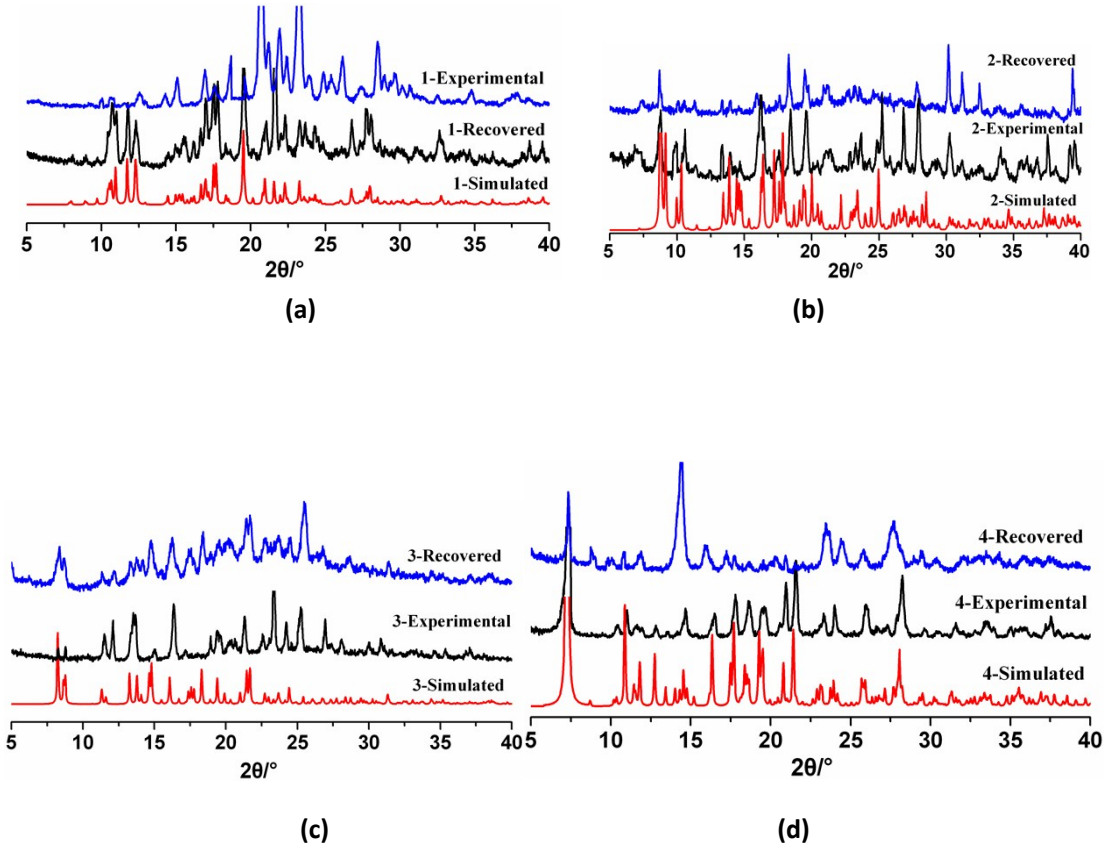
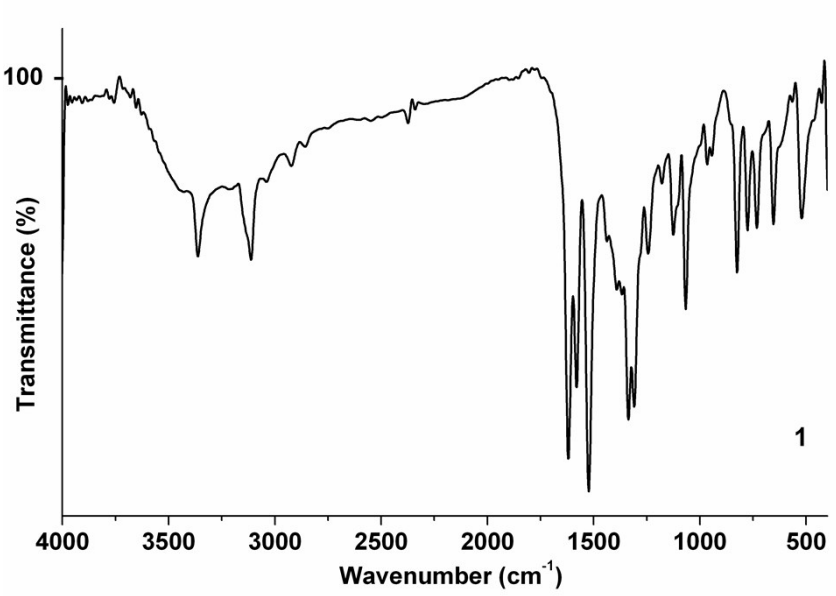


Fig. S1. (a) Powder XRD patterns of bulk sample of **1** (up) and Rietveld refinement of model determined by single crystal diffraction (down); (b) Powder XRD patterns of bulk sample of **2** (up) and Rietveld refinement of model determined by single crystal diffraction (down). (c) Powder XRD patterns of bulk sample of **3** (up) and Rietveld refinement of model determined by single crystal diffraction (down); (d) Powder XRD patterns of bulk sample of **4** (up) and Rietveld refinement of model determined by single crystal diffraction (down).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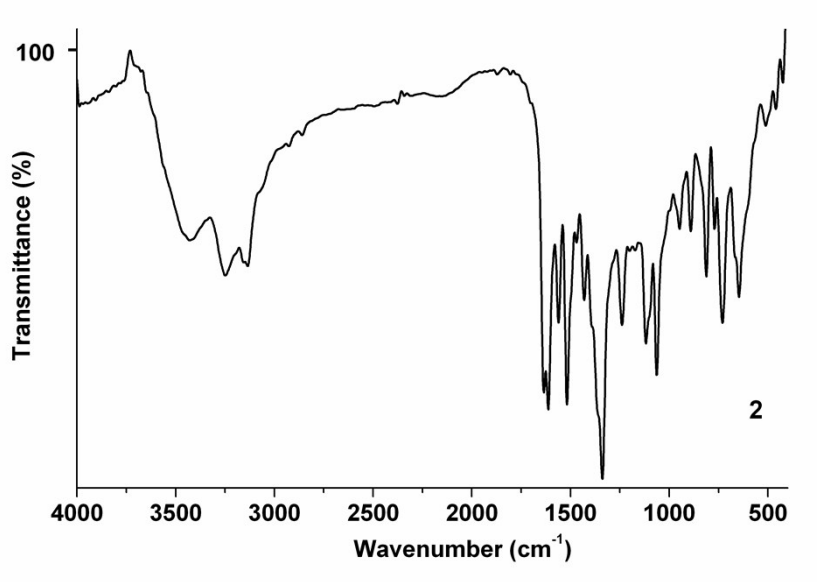
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

(a)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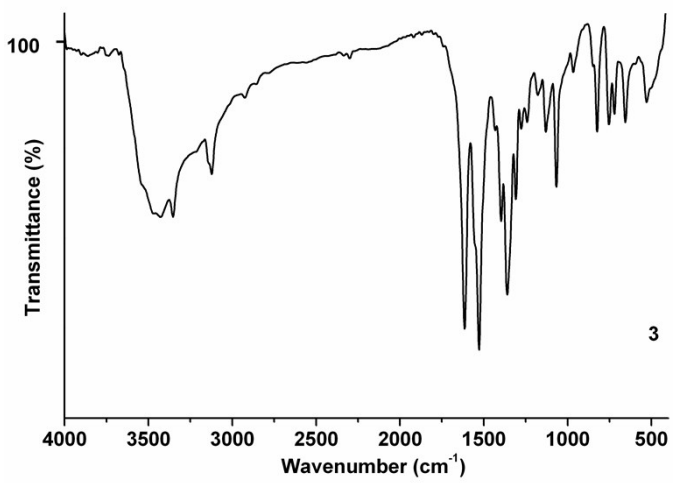
Wavenumber (cm-1)

(b)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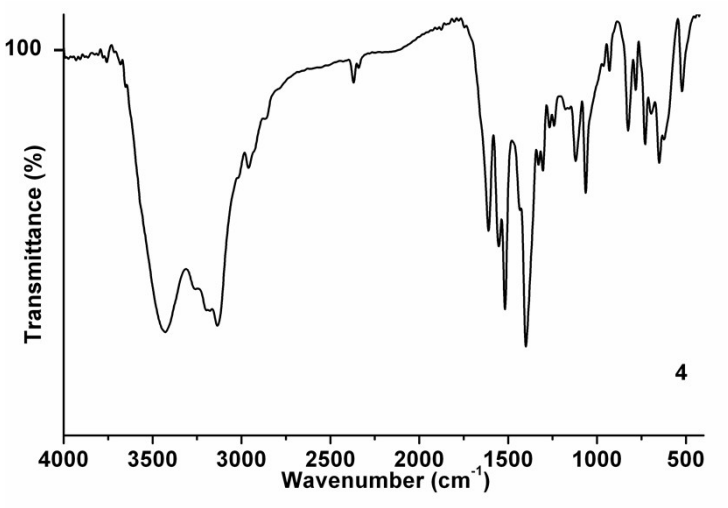
(c)



(d)

Figure S2. (a) FTIR spectraum for compound **1**. (b) FTIR spectraum for compound **2**. (c) FTIR spectraum for compound **3**. (d) FTIR spectraum for compound **4**.

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

Complex **1**			
Zn(1)-N(1)	2.038(9)	Zn(1)-N(5A)	2.008(9)
Zn(2)-N(10B)	2.003(15)	Zn(2)-N(6)	2.029(9)
Zn(1)-O(1)	1.953(7)	Zn(1)-O(5)	1.990(7)
Zn(2)-O(7C)	1.944(7)	Zn(2)-O(3)	1.983(7)
O(1)-Zn(1)-O(5)	104.7(3)	O(1)-Zn(1)-N(5A)	132.0(4)
O(5)-Zn(1)-N(5A)	106.9(4)	O(1)-Zn(1)-N(1)	102.8(4)
O(5)-Zn(1)-N(1)	102.1(4)	N(5A)-Zn(1)-N(1)	104.9(4)
O(7C)-Zn(2)-N(10B)	124.8(4)	O(7C)-Zn(2)-O(3)	101.9(3))
N(10B)-Zn(2)-O(3)	111.2(5)	O(7C)-Zn(2)-N(6)	105.5(4)
N(10B)-Zn(2)-N(6)	108.5(4)	O(3)-Zn(2)-N(6)	101.8(4)
Complex **2**			
Cd(1)-N(1)	2.281(4)	Cd(2)-N(5)	2.233(4)
Cd(1)-O(2)	2.312(3)	Cd(1)-O(9)	2.330(3)
Cd(1)-O(10)	2.331(3)	Cd(1)-O(8B)	2.335(3)
Cd(1)-O(7B)	2.516(3)	Cd(1)-O(1)	2.590(3)
Cd(2)-O(5)	2.216(3)	Cd(2)-O(12)	2.385(3)
Cd(2)-O(4A)	2.347(4)	Cd(2)-O(3A)	2.501(3)
Cd(2)-O(11)	2.394(3)		
N(1)-Cd(1)-O(2)	88.25(12)	N(1)-Cd(1)-O(9)	172.84(13)
O(2)-Cd(1)-O(9)	84.76(10)	N(1)-Cd(1)-O(10)	94.25(14)
O(2)-Cd(1)-O(10)	136.26(11)	O(9)-Cd(1)-O(10)	91.89(12)
N(1)-Cd(1)-O(8B)	96.83(14)	O(2)-Cd(1)-O(8B)	139.12(11)

O(9)-Cd(1)-O(8B)	87.47(11)	O(10)-Cd(1)-O(8B)	83.98(12)
N(1)-Cd(1)-O(7B)	89.93(14)	O(2)-Cd(1)-O(7B)	85.90(9)
O(9)-Cd(1)-O(7B)	88.01(11)	O(10)-Cd(1)-O(7B)	137.67(11)
O(8B)-Cd(1)-O(7B)	53.71(11)	N(1)-Cd(1)-O(1)	92.05(13)
O(2)-Cd(1)-O(1)	52.71(10)	O(9)-Cd(1)-O(1)	84.98(10)
O(10)-Cd(1)-O(1)	83.55(11)	O(8B)-Cd(1)-O(1)	165.18(12)
O(7B)-Cd(1)-O(1)	138.45(9)	O(5)-Cd(2)-N(5)	136.46(13)
O(5)-Cd(2)-O(4A)	82.65(11)	N(5)-Cd(2)-O(4A)	140.75(13)
O(5)-Cd(2)-O(12)	85.43(11)	N(5)-Cd(2)-O(12)	88.98(12)
O(4A)-Cd(2)-O(12)	91.68(12)	O(5)-Cd(2)-O(11)	92.99(11)
N(5)-Cd(2)-O(11)	86.90(13)	O(4A)-Cd(2)-O(11)	95.71(13)
O(12)-Cd(2)-O(11)	172.18(12)	O(5)-Cd(2)-O(3A)	134.68(12)
N(5)-Cd(2)-O(3A)	88.38(13)	O(4A)-Cd(2)-O(3A)	53.69(11)
O(12)-Cd(2)-O(3A)	105.24(10)	O(11)-Cd(2)-O(3A)	81.30(11)
Complex **3**			
Zn(1)-N(1)	1.993(2)	Zn(1)-N(5A)	1.982(3)
Zn(1)-O(1)	1.942(2)	Zn(1)-O(3B)	1.954(2)
O(1)-Zn(1)-O(3B)	102.27(10)	O(1)-Zn(1)-N(5A)	117.30(12)
O(3B)-Zn(1)-N(5A)	109.52(12)	O(1)-Zn(1)-N(1)	100.00(10)
O(3B)-Zn(1)-N(1)	114.82(10)	N(5A)-Zn(1)-N(1)	112.48(11)
Complex **4**			
Cd(1)-N(1)	2.358(4)	Cd(1)-N(5A)	2.286(3)
Cd(1)-O(1)	2.365(3)	Cd(1)-O(4B)	2.339(3)
Cd(1)-O(2C)	2.363(3)	Cd(1)-O(3B)	2.534(3)
Cd(1)-O(2)	2.635(3)		
N(5A)-Cd(1)-O(4B)	145.35(11)	N(5A)-Cd(1)-N(1)	90.12(12)
O(4B)-Cd(1)-N(1)	86.63(12)	N(5A)-Cd(1)-O(2C)	88.57(11)
O(4B)-Cd(1)-O(2C)	93.54(11)	N(1)-Cd(1)-O(2C)	177.93(11)
N(5A)-Cd(1)-O(1)	130.61(12)	O(4B)-Cd(1)-O(1)	82.70(10)
N(1)-Cd(1)-O(1)	79.99(12)	O(2C)-Cd(1)-O(1)	102.07(11)
N(5A)-Cd(1)-O(3B)	91.63(11)	O(4B)-Cd(1)-O(3B)	53.73(10)
O(1)-Cd(1)-O(3B)	134.23(10)	N(5A)-Cd(1)-O(2)	83.69(11)
O(4B)-Cd(1)-O(2)	130.71(9)	N(1)-Cd(1)-O(2)	101.94(12)
O(2C)-Cd(1)-O(2)	79.51(10)	O(1)-Cd(1)-O(2)	52.29(9)
O(3B)-Cd(1)-O(2)	172.59(9)	O(2C)-Cd(1)-O(3B)	94.68(10)
N(1)-Cd(1)-O(3B)	83.76(12)		

[a] Symmetry codes: (A) $x + 1, y + 1, z$; (B) $x + 1, y - 1, z$; (C) $x + 1/2, -y, z + 1/2$ for **1**. (A) $-x + 3, -y + 1, -z + 2$; (B) $-x + 2, -y, -z + 2$ for **2.** (A) $x - 1, y + 1, z$; (B) $-x + 1, y + 1/2, -z + 3/2$. for **3**. (A) $x, y + 1, z$; (B) $-x + 1, -y + 1, -z + 1$; (C) $x - 1, y, z$ for **4**.

Table S2. Hydrogen-bonding interactions in **1**-**4**.

Interaction	D–H [Å]	H···A [Å]	D···A [Å]	Angle (D–H···A) [°]
Complex **1**				
N3–H3A···O5[a]	0.86	2.52	3.36(2)	164
N8–H8A···O3[b]	0.86	2.43	3.27(2)	165.0
Symmetry codes: *a*, *x* − 1, *y*, *z*; *b*, *x*, *y* + 1, z.				
Complex **2**				
O9–H9B···O4[a]	1.07	1.76	2.811(4)	165.03
O9–H9C···O5[b]	0.82	1.97	2.781(4)	170.3
O10–H10A···O1[c]	0.82	1.96	2.759(4)	164.8
O10–H10B···O13[d]	1.04	2.13	3.151(4)	165.3
O11–H11B···O13[e]	0.90	2.13	3.017(4)	167.3
O11–H11C···O6[e]	0.82	1.97	2.759(5)	162.6
O12–H12B···O2[f]	0.82	1.92	2.738(4)	179.6
O12–H12C···O7[g]	0.93	1.88	2.807(4)	171.1
O13–H13A···O8	0.85	1.85	2.663(4)	159.6
O13–H13B···O3[h]	0.85	1.95	2.740(4)	153.2
N3–H3A···O13[i]	0.86	2.110	2.943(5)	165.2
Symmetry codes: *a*, − *x* + 2, − *y* + 2, − *z* + 2; *b*, *x* − 1, *y* + 1, *z* ; *c*, − *x* + 2, − *y* + 1 , − *z* + 2; *d*, − *x* + 2, − *y*, − *z* + 2; *e*, − *x* + 3, − *y*, − *z* + 2; *f*, *x* + 1, *y* − 1, *z*; *g*, − *x* + 3, − *y* − 1, − *z* + 2; *h*, *x*, *y* − 1, *z*; *i*, − *x* + 5/2, − *y* + 1/2, − *z* + 3/2.				
Complex **3**				
O5–H5B···O3 [a]	0.85(6)	2.18	3.027(4)	179.1
O5–H5C···O6	0.85	1.96	2.772(5)	160.1
O6–H6B···O2[b]	0.85	1.95	2.784(4)	168.0
O6–H6C···O3[c]	0.86	2.06	2.913(4)	175.8
N3–H3A···O5[e]	0.86	1.90	2.713(9)	157.9
Symmetry codes: *a*, − *x* + 1, − *y* + 1, − *z* + 1; *b*, − *x* + 1, − *y* + 2, − *z* + 1 ; *c*, *x*, − *y* + 3/2, *z* − 1.				
Complex **4**				
O5–H5C···O1	0.85	2.14	2.922(6)	153.7
O5–H5D···O4[a]	0.85	1.96	2.804(6)	173.5
N3–H3A···O3b[b]	0.86	2.18	2.934(5)	145.9
Symmetry codes: *a*, *x* − 1, *y*, *z*; *b*, − *x* + 1, *y* − 1/2, − *z* + 1/2.				

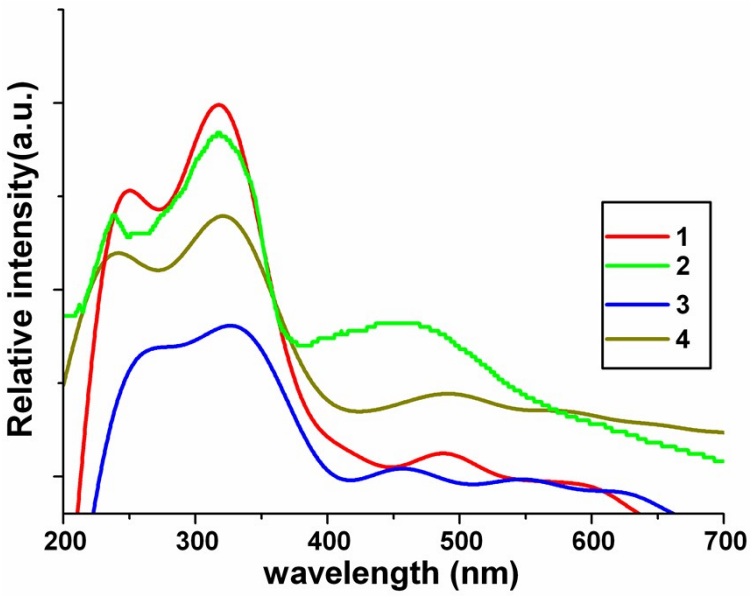


Fig. S3 The UV-vis absorption spectra for **1**–**4** in the solid state at room temperature

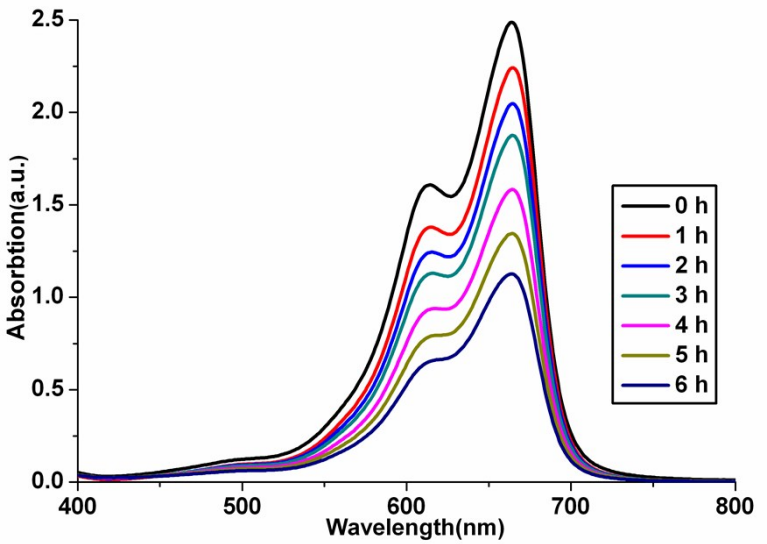


Fig. S4 UV-Vis absorption spectra of a MB solution degraded without catalysts under UV irradiation at different time intervals

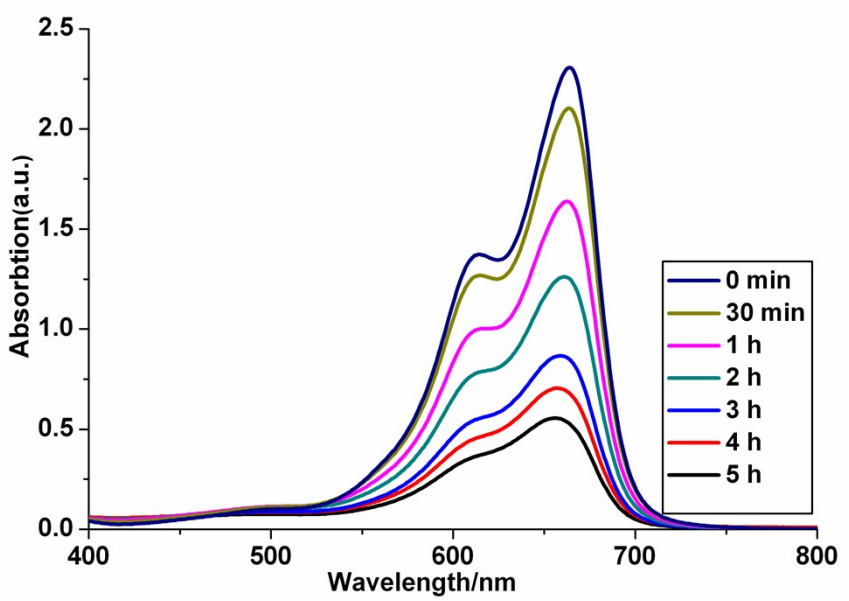


Fig. S5 UV-Vis absorption spectra of the MB solutions degraded by **1** under UV irradiation at different time intervals.

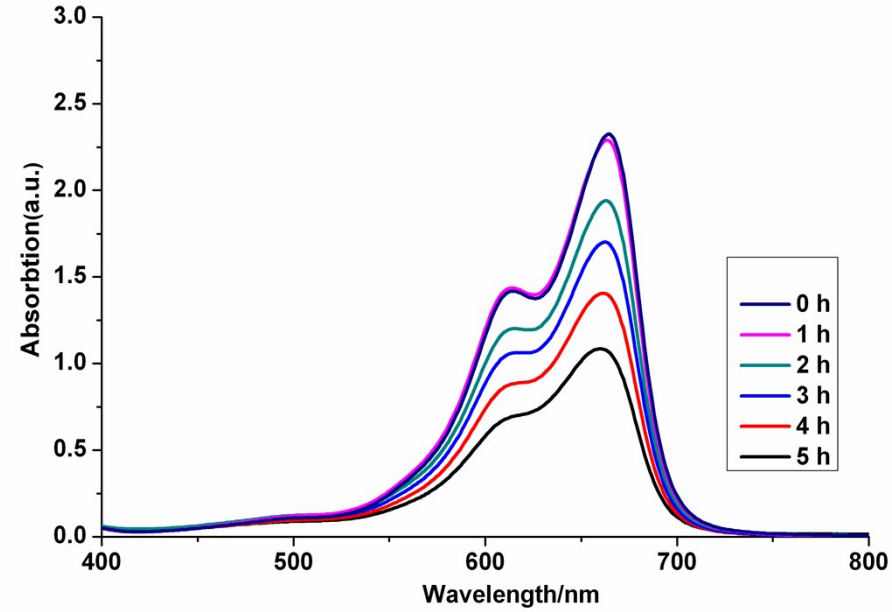


Fig. S6 UV-Vis absorption spectra of the MB solutions degraded by **3** under UV irradiation at different time intervals.

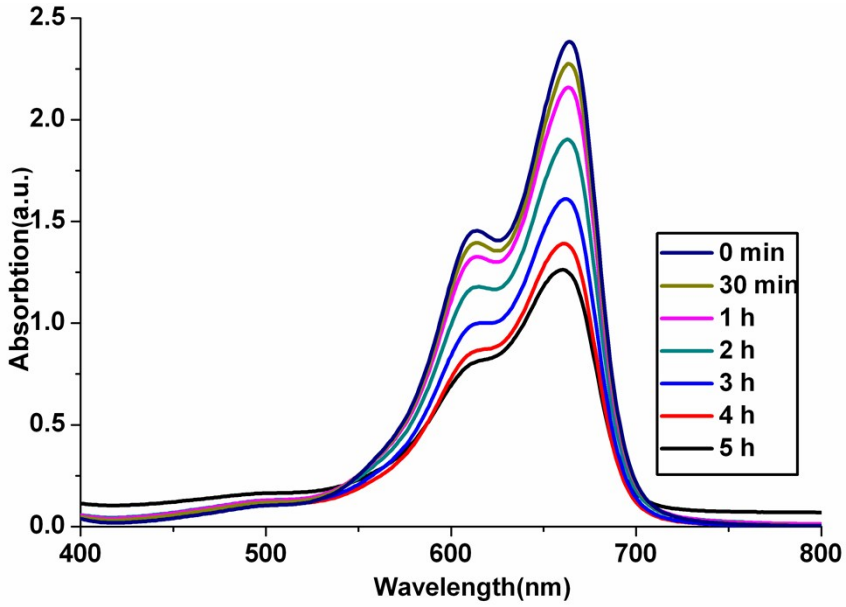
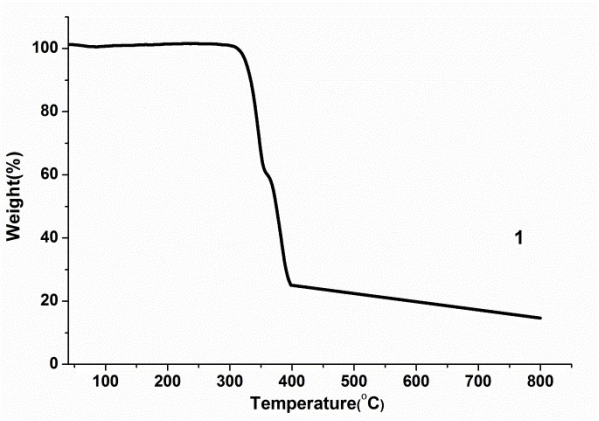
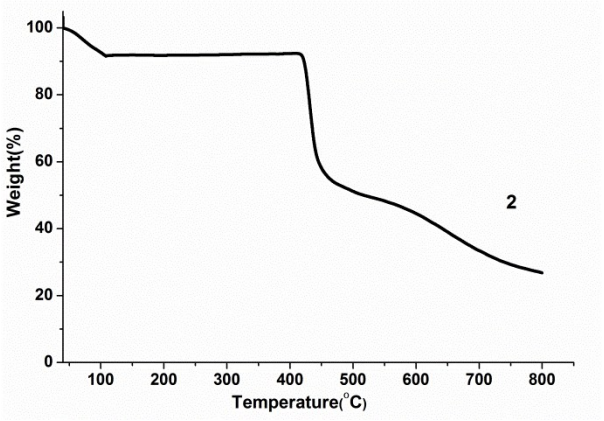


Fig. S7 UV-Vis absorption spectra of the MB solutions degraded by **4** under UV irradiation at different time intervals.



(a)



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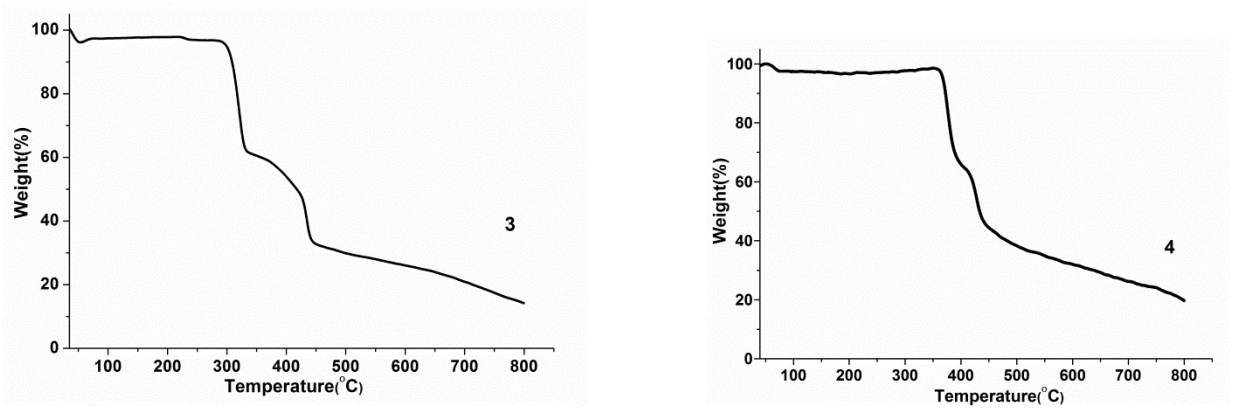

(c) (d)

Figure S8. (a) The TGA curves for **1**; (b) The TGA curves for **2**; (c) The TGA curves for **3** and (d) The TGA curves for **4**.