Supporting Information

Coordinate bond- and hydrogen bond-assisted electron transfer strategy towards the generation of photochromic metal phosphites based on nonphotoactive polypyridine units

Ai-Ju Liu, Yue Han, Fei Xu, Song-De Han*, Jie Pan, Guo-Ming Wang*

College of Chemistry and Chemical Engineering, Qingdao University, Shandong 266071, P. R. China.

*Author to whom correspondence should be addressed. E-mail: hansongde@yeah.net (S.-D. Han), gmwang_pub@163.com (G.-M. Wang)

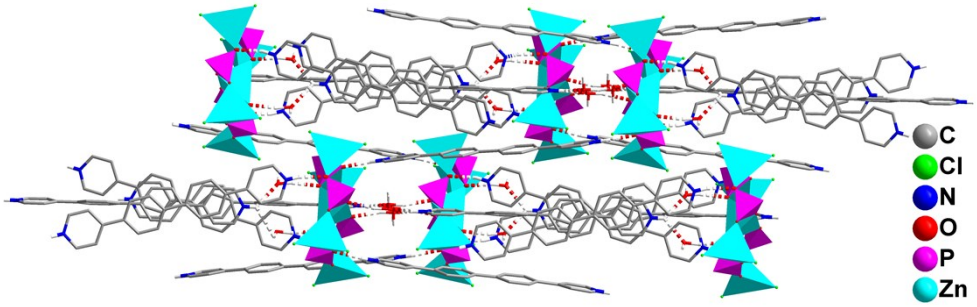

Fig. S1 The hydrogen bond-driven supramolecular extended structure of **2** with H-bonds shown as dashed lines.

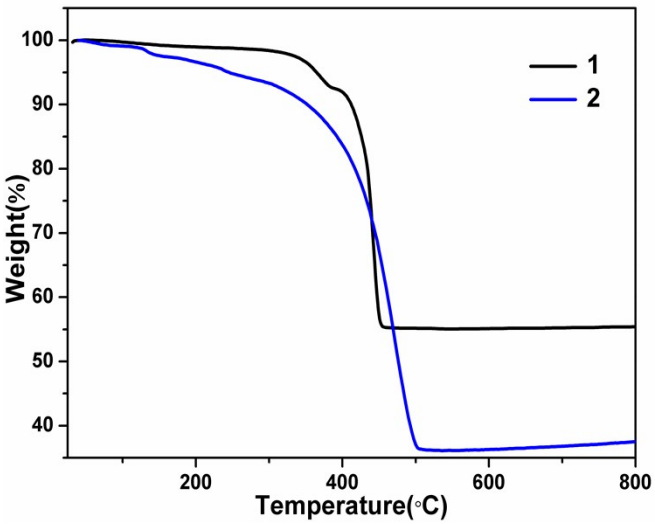

Fig. S2 The TG plots of **1** and **2**.

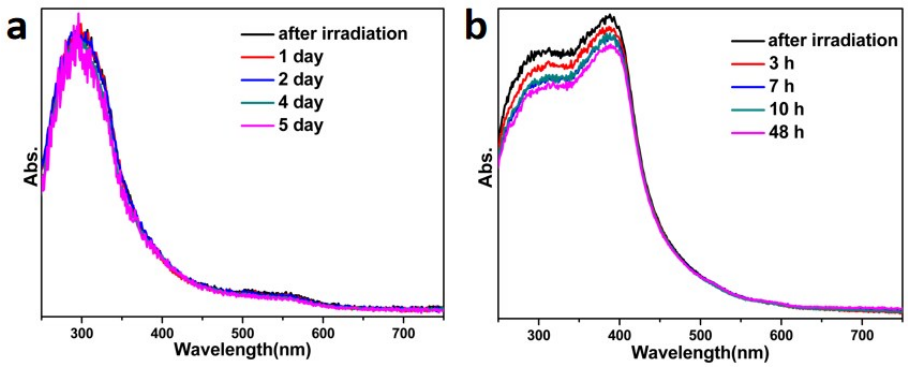

Fig. S3 Time-dependent UV-Vis spectra of colored sample of **1** (a) and **2** (b) via putting the corresponding sample in darkness.

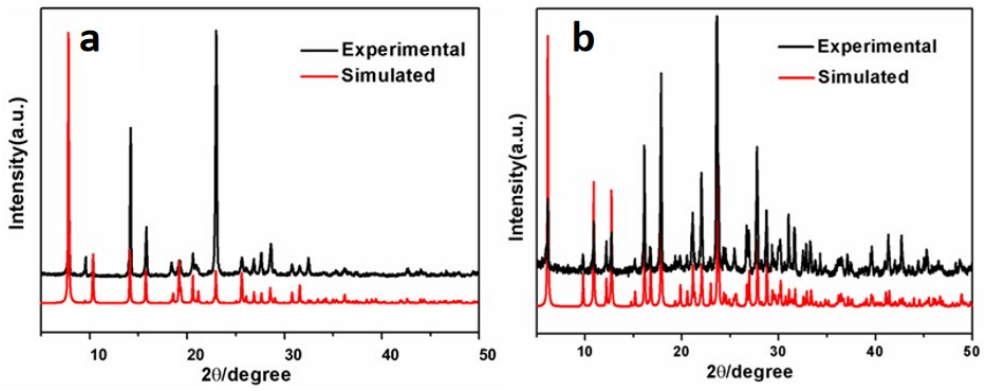

Fig. S4 PXRD patterns of the photoactivated sample of **1** (left) and **2** (right).

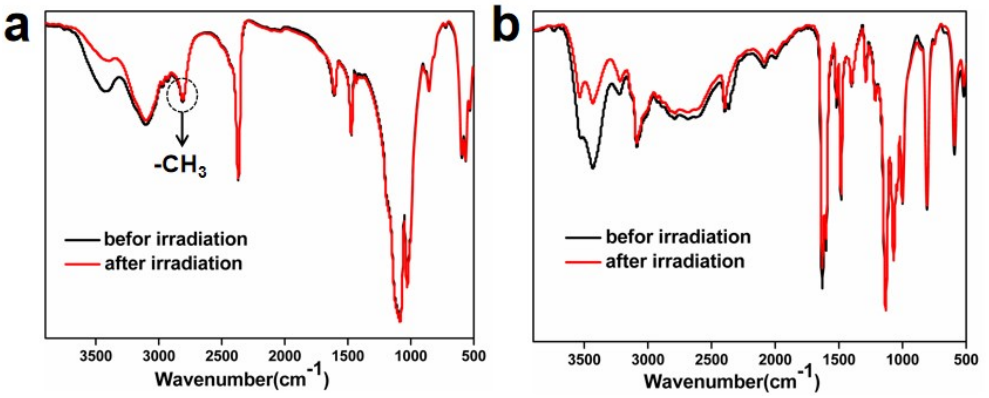

Fig. S5 IR patterns of **1** (a) and **2** (b).

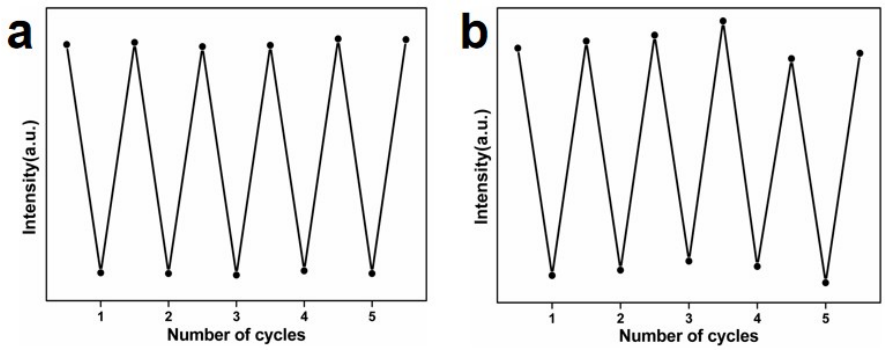

Fig. S6 Recycle results of photoluminescence for **1** (a) excited at 280 nm and **2** (b) excited at 280 nm via alternatively conducting Xe-lamp irradiation and heating treatments.

Table S1. SHAPE analysis of the Zn(II) ions in **1** and **2**

Metal	Label	Shape	Symmetry	Distortion
1-Zn1	SP-4	Square	D_{4h}	31.645
1-Zn1	T-4	Tetrahedron	T_d	0.262
1-Zn1	SS-4	Seesaw	C_{2V}	8.107
2-Zn1	SP-4	Square	D_{4h}	29.324
2-Zn1	T-4	Tetrahedron	T_d	0.938
2-Zn1	SS-4	Seesaw	C_{2V}	6.526
2-Zn2	SP-4	Square	D_{4h}	31.580
2-Zn2	T-4	Tetrahedron	T_d	0.035
2-Zn2	SS-4	Seesaw	C_{2V}	9.055

Table S2. Selected bond lengths (Å) and angles (°) for **1**

Zn(1)-O(3)#1	1.904(2)	P(1)-O(1)	1.497(2)
Zn(1)-O(2)#2	1.916(3)	P(1)-O(2)	1.500(3)
Zn(1)-O(1)	1.922(2)	P(1)-O(3)	1.503(3)
Zn(1)-N(1)	2.045(3)		
O(3)#1-Zn(1)-O(2)#2	114.05(13)	O(1)-Zn(1)-N(1)	107.95(13)
O(3)#1-Zn(1)-O(1)	109.62(11)	O(1)-P(1)-O(2)	114.53(16)
O(2)#2-Zn(1)-O(1)	116.92(11)	O(1)-P(1)-O(3)	110.72(15)
O(3)#1-Zn(1)-N(1)	106.12(12)	O(2)-P(1)-O(3)	113.41(16)
O(2)#2-Zn(1)-N(1)	101.11(12)		

Symmetry codes: #1: x, y+1, z; #2: -x+5/2, y+1/2, -z+1/2; #3: -x+1, -y+1, -z; #4: -x+5/2, y-1/2, -z+1/2; #5: x, y-1, z.

Table S3. Selected bond lengths (Å) and angles (°) for **2**

Zn(1)-O(1)	1.917(3)	Zn(1)-Cl(2)	2.2242(13)
Zn(1)-O(2)	1.958(3)	P(1)-O(1)#4	1.492(3)
Zn(2)-O(3)	1.945(3)	P(1)-O(2)	1.515(3)
Zn(1)-Cl(1)	2.2274(13)	P(1)-O(3)	1.512(3)
O(1)-Zn(1)-Cl(2)	105.52(11)	O(3)-Zn(2)-O(3)#5	108.41(8)
O(2)-Zn(1)-Cl(2)	109.40(9)	O(3)-Zn(2)-O(3)#4	108.40(8)
O(1)-Zn(1)-Cl(1)	110.94(12)	O(3)-Zn(2)-O(3)#6	111.62(16)
O(2)-Zn(1)-Cl(1)	101.43(9)	O(3)#5-Zn(2)-O(3)#6	108.41(8)
Cl(2)-Zn(1)-Cl(1)	118.56(5)	O(1)#5-P(1)-O(3)	114.89(19)
O(1)-Zn(1)-O(2)	111.02(14)	O(1)#5-P(1)-O(2)	108.66(18)
O(3)-Zn(2)-O(3)#5	108.41(8)	O(3)-P(1)-O(2)	113.49(17)
O(3)-Zn(2)-O(3)#6	111.61(16)		

Symmetry codes: #1: -x+1/2, -y+1/2, -z+1/2; #2: -x+2, -y+1/2, z+0; #3: y+3/4, -x+5/4, -z+9/4; #4: y-1/4, -x+5/4, -z+1/4; #5: -y+5/4, x+1/4, -z+1/4; #6: -x+1, -y+3/2, z+0.

Table S4 Details of selected hydrogen bond in **2**

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (deg)
O4-H4A···O3_$1	0.96	1.86	2.803(6)	167
O4-H4B···Cl1_$2	0.96	2.33	3.289(8)	175
N1-H1···O2_$3	0.86	1.91	2.756(6)	166
N2-H2A···O4	0.86	2.14	2.783(10)	132

Symmetry codes: $1: 1/4+y, 3/4-x, 3/4-z; $2: 1-x, 1-y, 1-z; $3: -1/4+y, 3/4-x, -1/4+z.