

# Supporting Information

**Effects of Metal Ions and *N*-Donor Ligands with Different Coordination Characters on the Construction of  $d^{10}$  Metal-organic Complexes with Selective Photocatalytic Activities**

Guo-Cheng Liu, Nai-Li Chen, Ju-Wen Zhang, Yun Qu, Hong-Yan Lin, and Xin-Jie Gao

Department of Chemistry, Bohai University, Liaoning Province Silicon Materials Engineering Technology Research Centre, Jinzhou, 121000, P. R. China

Table S1. Selected bond lengths (Å) and angles (deg) for compound **1**.

<b>1</b>			
Zn1–O1	1.9938(17)	Zn1–O3(A)	1.9988(18)
Zn1–O1W	2.1619(19)	Zn1–N1	2.1293(19)
Zn1–N2	2.166(2)		
O1–Zn1–O3(A)	132.63(7)	O1–Zn1–O1W	88.70(7)
O3(A)–Zn1–O1W	93.39(7)	O1–Zn1–N1	111.91(7)
O3(A)–Zn1–N1	115.45(7)	O1W–Zn1–N1	88.43(7)
O1–Zn1–N2	97.00(7)	O3(A)–Zn1–N2	92.15(7)
O1W–Zn1–N2	165.96(7)	N1–Zn1–N2	77.54(7)

Symmetry code: A:  $-x+1, y+1/2, -z+1/2$ .Table S2. Selected bond lengths (Å) and angles (deg) for compound **2**.

<b>2</b>			
Cd1–O1	2.2415(16)	Cd1–O3(A)	2.3110(17)
Cd1–O4(B)	2.3641(16)	Cd1–N2	2.3644(18)
Cd1–N1	2.3671(18)	Cd1–O4(A)	2.584(2)
Cd1–O2	2.644(2)		
O1–Cd1–O3(A)	129.88(7)	O1–Cd1–O4(B)	83.33(6)
O3(A)–Cd1–O4(B)	115.64(6)	O1–Cd1–N2	145.91(7)
O3(A)–Cd1–N2	84.20(6)	O4(B)–Cd1–N2	79.83(6)
O1–Cd1–N1	101.35(7)	O3(A)–Cd1–N1	97.19(6)
O4(B)–Cd1–N1	132.85(7)	N2–Cd1–N1	70.43(6)
O1–Cd1–O4(A)	96.58(6)	O3(A)–Cd1–O4(A)	52.57(5)
O4(B)–Cd1–O4(A)	73.58(7)	N2–Cd1–O4(A)	106.64(6)
N1–Cd1–O4(A)	149.35(6)	O1–Cd1–O2	52.43(6)
O3(A)–Cd1–O2	85.51(6)	O4(B)–Cd1–O2	131.06(6)
N2–Cd1–O2	148.64(6)	N1–Cd1–O2	81.62(6)
O4(A)–Cd1–O2	90.08(6)		

Symmetry code: A:  $x-1, y, z$ ; B:  $-x+3, -y+1, -z+1$ .

Table S3. Selected bond lengths (Å) and angles (deg) for compound **3**.

<b>3</b>			
Zn1–O1	1.958(3)	Zn1...O2	2.826(3)
Zn1–N1	2.080(2)	Zn1–N5(A)	2.083(2)
Zn1–O3(B)	2.290(3)	Zn1–O4(B)	2.108(2)
O1–Zn1–N5(A)	94.52(10)	O1–Zn1–N1	106.53(11)
N5(A)–Zn1–N1	103.70(9)	O1–Zn1–O4(B)	101.51(11)
N5(A)–Zn1–O4(B)	98.72(9)	N1–Zn1–O4(B)	142.21(10)
N5(A)–Zn1–O3(B)	91.24(9)	N1–Zn1–O3(B)	90.19(9)
O4(B)–Zn1–O3(B)	59.04(9)	O1–Zn1–O3(B)	160.40(10)

Symmetry code: A:  $x+1/2, -y+1/2, z-1/2$ ; B:  $x+1, y, z$ .Table S4. Selected bond lengths (Å) and angles (deg) for compound **4**.

<b>4</b>			
Cd1–O3(A)	2.300(4)	Cd1–O4(A)	2.400(3)
Cd1–N1	2.295(3)	Cd1–N5(B)	2.323(3)
Cd1–O1	2.297(2)	Cd1–O2	2.428(2)
N1–Cd1–O1	140.39(10)	N1–Cd1–O3(A)	121.95(18)
O1–Cd1–O3(A)	95.49(17)	N1–Cd1–N5(B)	97.05(10)
O1–Cd1–N5(B)	99.47(9)	O3(A)–Cd1–N5(B)	84.01(11)
N1–Cd1–O4(A)	90.56(11)	O1–Cd1–O4(A)	102.66(11)
O3(A)–Cd1–O4(A)	54.79(12)	N5(B)–Cd1–O4(A)	134.46(11)
N1–Cd1–O2	90.14(9)	O1–Cd1–O2	55.42(9)
O3(A)–Cd1–O2	147.42(17)	N5(B)–Cd1–O2	86.70(9)
O4(A)–Cd1–O2	138.31(11)		

Symmetry code: A:  $1+x, y, z$ ; B:  $-1/2+x, 1/2-y, 1/2+z$ .

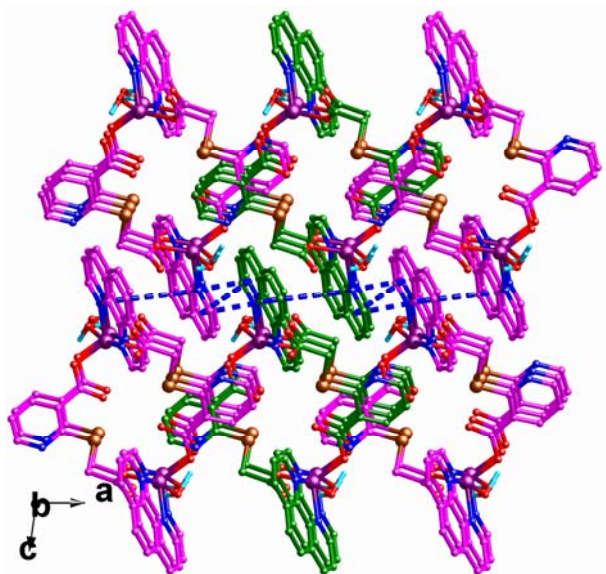


Fig. S1. 3-D supramolecular framework of **1**.

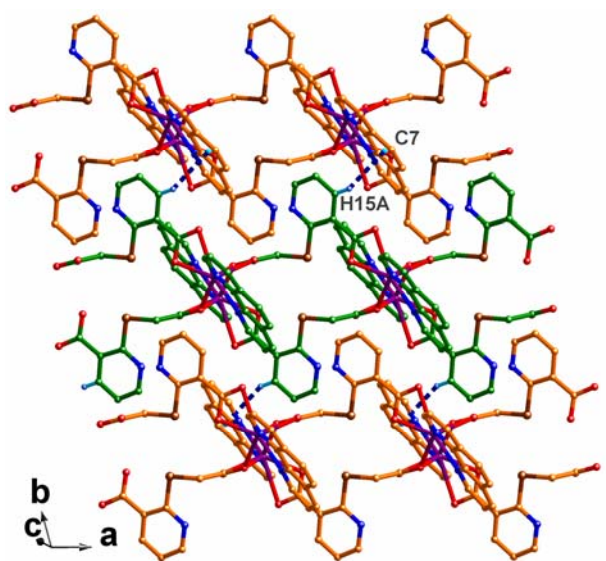


Fig. S2. Supramolecular layer connected by C-H... $\pi$  interactions of **2**.

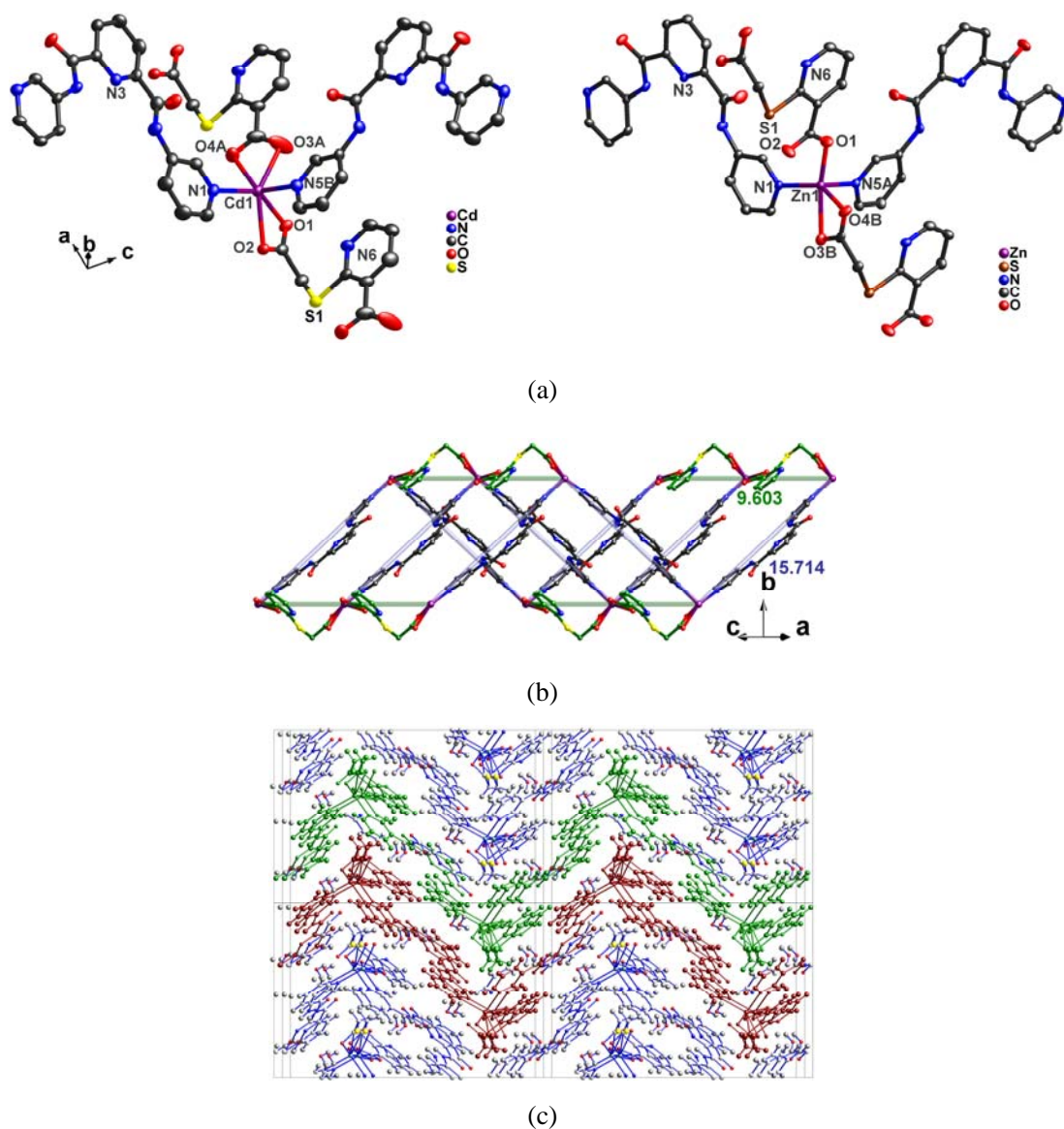


Fig. S3. (a) The coordination environment of the Cd<sup>II</sup> ion in compound **4** (A:  $1+x, y, z$ ; B:  $-1/2+x, 1/2-y, 1/2+z$ ) (left) and the Zn<sup>II</sup> ion in compound **3** (right); (b) view of the wave-like network in **4**; (c) 3-D supramolecular framework derived from layers bridged by hydrogen bonding interactions in **4** (N2–H2A $\cdots$ O1W = 3.068(4) Å, 148°; O2W–H2WA $\cdots$ O2(C) = 2.850(5) Å, 171°; O2W–H2WB $\cdots$ O5(C) = 2.969(5) Å, 167°; C:  $-1+x, y, z$ ; N4–H4B $\cdots$ O1W = 3.033(4) Å, 155°).

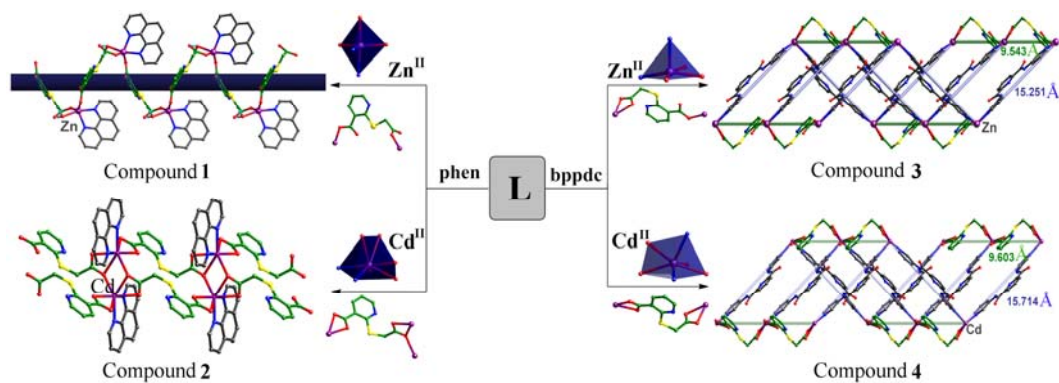


Fig. S4. Schematic view of the effects of N-donor ligands and metal ions on the L-based coordination polymers **1–4**.

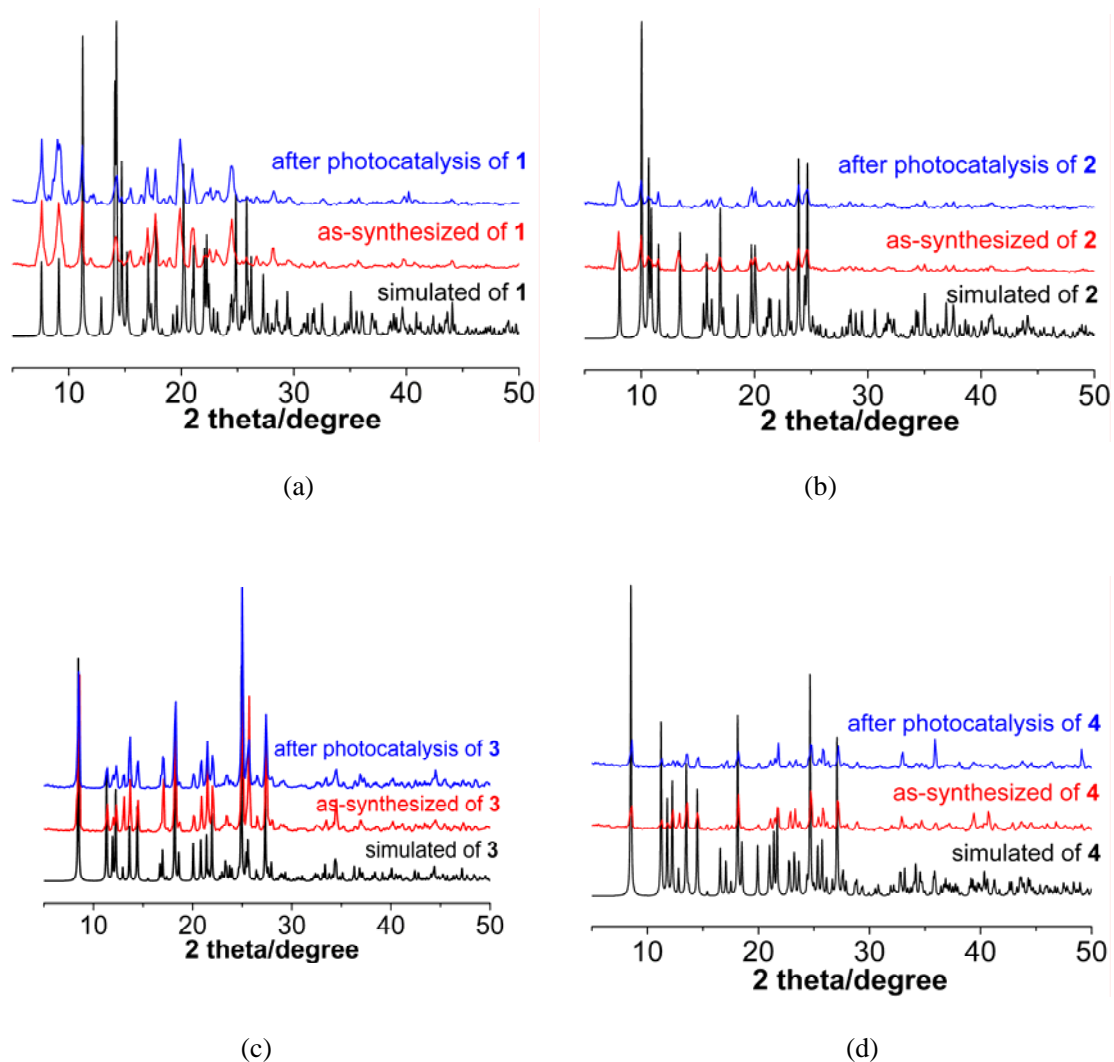
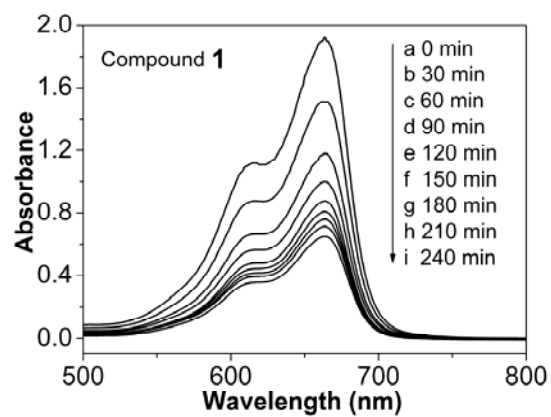
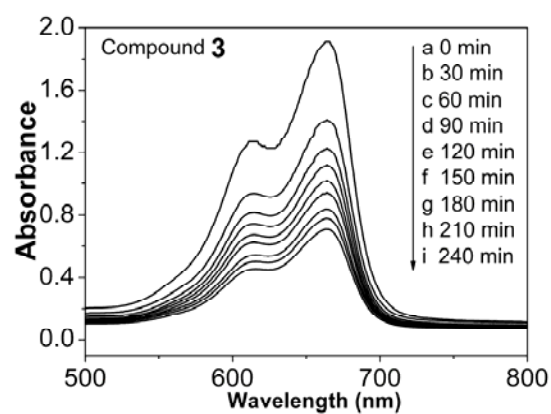


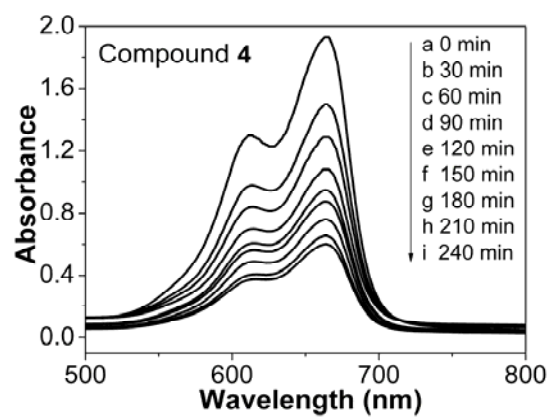
Fig. S5. Simulated (black) and experimental (red) PXRD patterns for compounds **1–4**, the PXRD patterns of compounds **1–4** after photocatalytic processes (blue).



(a)



(b)



(c)

Fig. S6. Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation with the use of compounds **1** (a), **3** (b) and **4** (c).