Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Metal-dependent photochromic performance in two isostructural supramolecular chains

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Instruments used in this work

Elemental analyses (EA) were characterised on a Perkin-Elmer 2400 elemental analyzer. Thermogravimetric analyses (TGA) were characterised on a Perkin-Elmer TGA-7 thermogravimetric analyzer. IR analyses were characterised on a Bruker VECTOR 22 spectrometer. The luminescent analyses were characterised on an F-4700 FL spectrophotometer. The UV-Vis analyses were characterised on a Varian Cary 500 UV-Vis spectrophotometer. Electron paramagnetic resonance (EPR) analyses were characterised on Bruker EMX spectrometer. The photoirradiation course was completed with a Perfect Light PLS-SXE 300 (300 W). The powder X-ray diffraction (PXRD) analyses were characterised on a Rigaku D/max-2550 diffractometer with Cu-K_α radiation (λ = 1.5418 Å). The data for fitting the PXRD curve were extracted from the single-crystal XRD (SCXRD) data via Mercury.

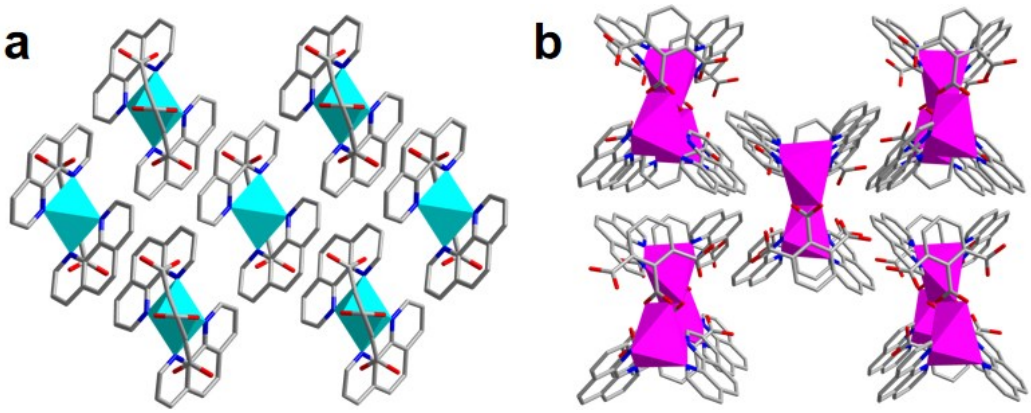

Fig. S1 The packing structures of **1** (a) and **2** (b).

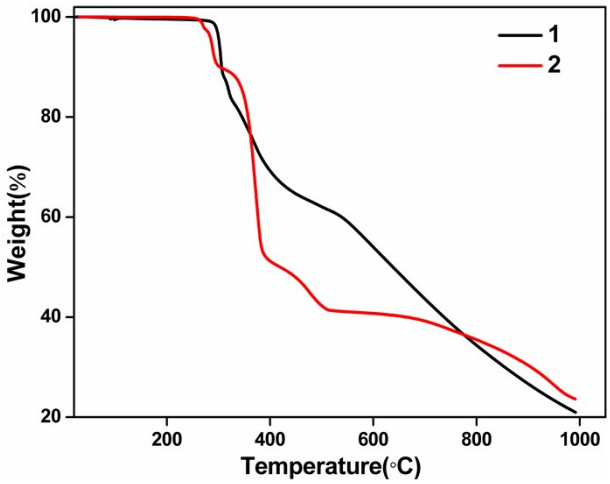

Fig. S2 The TG plots of **1** and **2**.

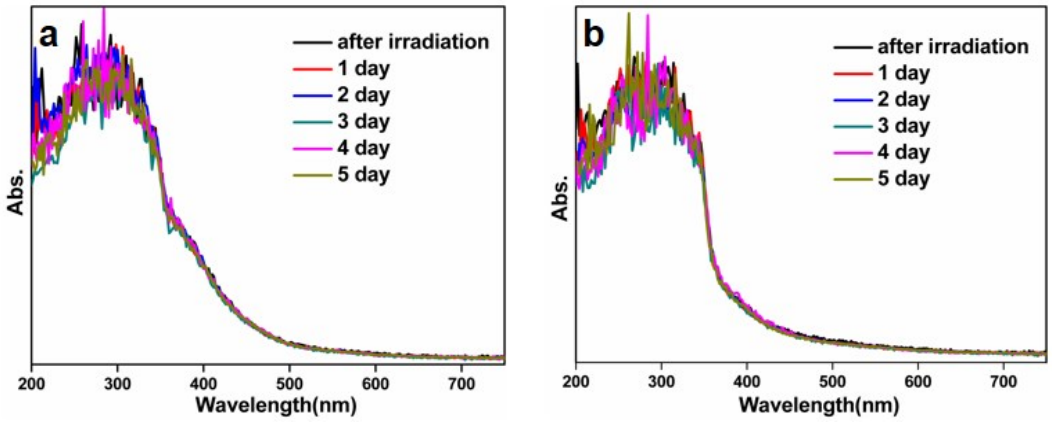

Fig. S3 Time-dependent UV-Vis spectra of colored sample of **1** (a) and **2** (b) via putting the photoactivated samples in darkness.

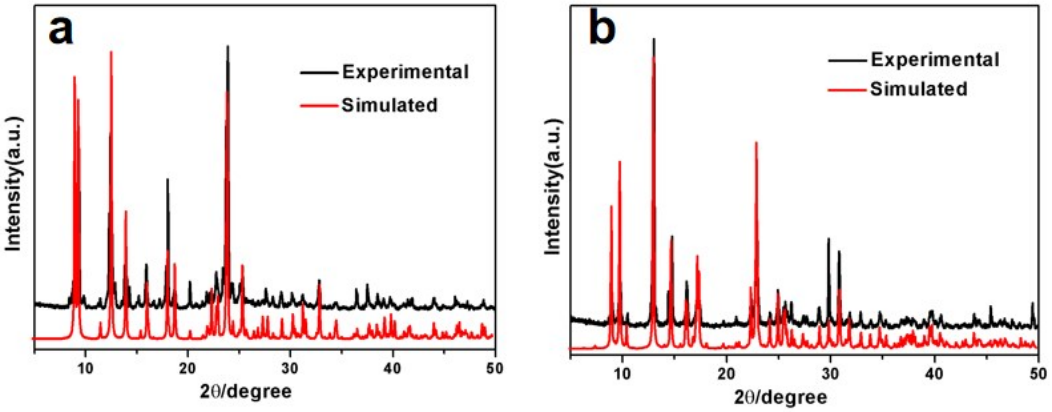

Fig. S4 PXRD patterns of the photoactivated sample of **1** (a) and **2** (b).

Table S1 Selected bond lengths (Å) and angles (°) for **1**

Zn(1)-N(1)	2.0937(16)	Zn(1)-O(1)#1	2.1703(13)
Zn(1)-N(1)#1	2.0937(16)	Zn(1)-N(2)	2.1910(16)
Zn(1)-O(1)	2.1703(13)	Zn(1)-N(2)#1	2.1910(15)
N(1)-Zn(1)-N(1)#1	159.58(9)	O(1)-Zn(1)-O(1)#1	60.35(7)
N(1)-Zn(1)-O(1)	99.23(6)	N(1)-Zn(1)-N(2)	77.65(6)
N(1)#1-Zn(1)-O(1)	98.40(6)	N(1)#1-Zn(1)-N(2)	87.96(6)
N(1)-Zn(1)-O(1)#1	98.41(6)	O(1)-Zn(1)-N(2)	164.41(5)
N(1)#1-Zn(1)-O(1)#1	99.23(6)	O(1)#1-Zn(1)-N(2)	104.69(5)
N(1)-Zn(1)-N(2)#1	87.95(6)	N(1)#1-Zn(1)-N(2)#1	77.65(6)
O(1)-Zn(1)-N(2)#1	104.69(5)	O(1)#1-Zn(1)-N(2)#1	164.41(5)
N(2)-Zn(1)-N(2)#1	90.54(9)		

Symmetry codes:#1: -x+1, y, -z+1/2.

Table S2 Selected bond lengths (Å) and angles (°) for **2**

Cd(1)-O(3)	2.318(3)	Cd(2)-O(9)	2.373(3)
Cd(1)-O(4)	2.335(3)	Cd(2)-O(10)	2.276(3)
Cd(1)-N(1)	2.290(4)	Cd(2)-N(5)	2.293(4)
Cd(1)-N(4)	2.294(4)	Cd(2)-N(8)	2.301(4)
Cd(1)-N(3)	2.293(4)	Cd(2)-N(7)	2.343(4)
Cd(1)-N(2)	2.301(4)	Cd(2)-N(6)	2.374(4)
N(1)-Cd(1)-N(4)	156.03(16)	O(9)-Cd(2)-N(5)	101.05(14)
N(1)-Cd(1)-O(3)	103.57(13)	O(9)-Cd(2)-N(8)	103.15(14)
N(4)-Cd(1)-O(3)	95.62(13)	N(5)-Cd(2)-N(8)	154.43(17)
N(1)-Cd(1)-O(4)	102.76(13)	O(9)-Cd(2)-N(7)	154.79(13)
N(4)-Cd(1)-O(4)	99.77(14)	N(5)-Cd(2)-N(7)	89.43(15)
O(3)-Cd(1)-O(4)	56.40(12)	N(8)-Cd(2)-N(7)	71.86(14)
N(1)-Cd(1)-N(3)	94.12(14)	O(9)-Cd(2)-O(10)	56.10(12)
N(4)-Cd(1)-N(3)	72.08(14)	N(5)-Cd(2)-O(10)	97.45(13)
O(3)-Cd(1)-N(3)	156.49(13)	N(8)-Cd(2)-O(10)	102.79(14)
O(4)-Cd(1)-N(3)	104.94(12)	N(7)-Cd(2)-O(10)	100.12(13)
N(1)-Cd(1)-N(2)	71.69(14)	O(9)-Cd(2)-N(6)	109.18(13)
N(4)-Cd(1)-N(2)	89.74(15)	N(5)-Cd(2)-N(6)	71.71(14)
O(3)-Cd(1)-N(2)	104.86(12)	N(8)-Cd(2)-N(6)	92.50(15)
O(4)-Cd(1)-N(2)	159.47(13)	N(7)-Cd(2)-N(6)	95.84(17)
N(3)-Cd(1)-N(2)	95.26(14)	O(10)-Cd(2)-N(6)	160.65(14)

Table S3 SHAPE analysis of the metal ions in **1** and **2**

Metal	Label	Shape	Symmetry	Distortion
1-Zn1	HP-6	Hexagon	D_{6h}	25.431
1-Zn1	PPY-6	Pentagonal pyramid	C_{5v}	22.623
1-Zn1	OC-6	Octahedron	O_h	7.880
1-Zn1	TPR-6	Trigonal prism	D_{3h}	14.465
1-Zn1	JPPY-6	Johnson pentagonal pyramid J2	C_{5v}	26.452
2-Cd1	HP-6	Hexagon	D_{6h}	27.344
2-Cd1	PPY-6	Pentagonal pyramid	C_{5v}	21.004
2-Cd1	OC-6	Octahedron	O_h	5.122
2-Cd1	TPR-6	Trigonal prism	D_{3h}	10.735
2-Cd1	JPPY-6	Johnson pentagonal pyramid J2	C_{5v}	24.882
2-Cd2	HP-6	Hexagon	D_{6h}	27.554
2-Cd2	PPY-6	Pentagonal pyramid	C_{5v}	21.114
2-Cd2	OC-6	Octahedron	O_h	5.306
2-Cd2	TPR-6	Trigonal prism	D_{3h}	10.643
2-Cd2	JPPY-6	Johnson pentagonal pyramid J2	C_{5v}	24.752

Table S4 Details of selected hydrogen bond in **1**

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (deg)
O3-H3···O3	1.21	1.21	2.424(3)	180

Table S5 Details of selected hydrogen bond in **2**

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (deg)
O1-H1··O7	0.82	1.66	2.418(5)	152
O12-H12···O6	0.82	1.62	2.418(5)	164