Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

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Coordination-driven strategy towards crystalline hybrid photochromic materials via the marriage of non-photochromic extended dipyridine unit and zincophosphate

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Experimental Section

Materials and methods.

All chemicals were reagent grade and used as purchased without further purification.

Elemental analyses (C, H, and N) were measured on a Perkin-Elmer 240C analyzer (Perkin-Elmer, USA). IR spectra were performed on a MAGNA-560 (Nicolet) FT-IR spectrometer with KBr pellets. The luminescence data were recorded on an F-7000 FL spectrophotometer. The solid-state UV-Vis spectra were measured with powder samples on a PerkinElmer Lamda-950 spectrophotometer. Electron spin resonance (ESR) spectroscopy was recorded on a JEOL JES-FA200 EPR spectrometer. Powder X-ray diffraction (PXRD) spectra were recorded on a Bruker D8 FOCUS diffractometer with a Cu-target tube and a graphite monochromator. Simulation of the PXRD curve was carried out by the single-crystal data and diffraction-crystal module of the Mercury (Hg) program available free of charge *via* the Internet at http://www.iucr.org.

Synthesis of 1,4-di(pyridine-4-yl)benzene (bpyb)

bpyb was prepared according to literature procedure.[1]

X-ray Crystallography.

The single-crystal X-ray diffraction data of **1** and **2** were collected on an XtaLAB-mini diffractometer at 293(2) K with Mo-Kα radiation (λ = 0.71073 Å) and ω scan mode. SHELX-2016 software was used to solve the structure.[2] The selected bond lengths and angles are given in Table S1 and Table S2. Full crystallographic data for **1** and **2** have been deposited with the CCDC (1891504 and 1891505).

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

N(1)-Zn(1)	2.056(5)	O(5)-P(1)	1.536(3)
O(1)-Zn(1)#1	1.927(4)	O(6)-P(1)	1.522(4)
O(2)-Zn(1)	1.918(4)	O(1)-P(2)	1.511(4)
O(6)-Zn(1)	1.920(4)	O(2)-P(2)	1.521(4)
O(4)-Zn(2)	1.914(4)	O(3)-P(2)	1.575(4)
O(5)-Zn(2)	1.955(3)	O(4)-P(2)	1.510(4)
O(6)#2-P(1)-O(6)	112.8(3)	P(1)-O(6)-Zn(1)	123.2(2)
O(6)#2-P(1)-O(5)	106.80(18)	C(1)-N(1)-Zn(1)	122.3(4)
O(6)-P(1)-O(5)	110.35(19)	C(5)-N(1)-Zn(1)	120.4(4)
O(6)#2-P(1)-O(5)#2	110.35(19)	O(2)-Zn(1)-O(6)	115.66(16)
O(6)-P(1)-O(5)#2	106.80(18)	O(2)-Zn(1)-O(1)#1	112.28(16)
O(5)-P(1)-O(5)#2	109.7(3)	O(6)-Zn(1)-O(1)#1	109.30(16)
O(1)-P(2)-O(4)	109.6(2)	O(2)-Zn(1)-N(1)	99.97(18)
O(1)-P(2)-O(2)	112.9(2)	O(6)-Zn(1)-N(1)	111.18(17)
O(4)-P(2)-O(2)	113.3(2)	O(1)#1-Zn(1)-N(1)	107.92(17)
O(1)-P(2)-O(3)	107.1(2)	O(4)-Zn(2)-O(4)#3	116.4(3)
O(4)-P(2)-O(3)	108.3(2)	O(4)-Zn(2)-O(5)	119.69(15)
O(2)-P(2)-O(3)	105.2(2)	O(4)#3-Zn(2)-O(5)	95.64(14)
P(2)-O(1)-Zn(1)#1	123.1(2)	O(4)-Zn(2)-O(5)#3	95.63(14)
P(2)-O(2)-Zn(1)	130.4(2)	O(4)#3-Zn(2)-O(5)#3	119.69(15)
P(2)-O(4)-Zn(2)	137.1(2)	O(5)-Zn(2)-O(5)#3	111.5(2)
P(1)-O(5)-Zn(2)	126.3(2)		

Symmetry codes: #1 -*x*+1/2, -*y*+1, -*z*+3/2; #2 -*x*+3/4, -*y*+3/4, *z*; #3 *x*+3/4, *y*, *z*+7/4.

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

N(1)-Zn(1)	2.023(2)	O(1)-P(1)	1.523(2)
O(1)-Zn(1)	1.960(2)	O(2)-P(1)	1.568(2)
O(3)-Zn(1)#2	1.905(2)	O(3)-P(1)	1.516(2)
O(4)-Zn(1)#3	1.9061(19)	O(4)-P(1)	1.506(2)
O(4)-P(1)-O(3)	108.22(12)	C(1)-N(1)-Zn(1)	126.3(2)
O(4)-P(1)-O(1)	114.33(12)	C(5)-N(1)-Zn(1)	115.28(19)
O(3)-P(1)-O(1)	111.35(12)	O(3)#2-Zn(1)-O(4)#4	110.69(9)
O(4)-P(1)-O(2)	109.52(12)	O(3)#2-Zn(1)-O(1)	110.79(10)
O(3)-P(1)-O(2)	109.54(13)	O(4)#4-Zn(1)-O(1)	109.51(9)
O(1)-P(1)-O(2)	103.76(12)	O(3)#2-Zn(1)-N(1)	118.73(10)
P(1)-O(1)-Zn(1)	126.38(13)	O(4)#4-Zn(1)-N(1)	103.01(9)
P(1)-O(3)-Zn(1)#2	131.80(13)	O(1)-Zn(1)-N(1)	103.52(9)
P(1)-O(4)-Zn(1)#3	141.44(14)		

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

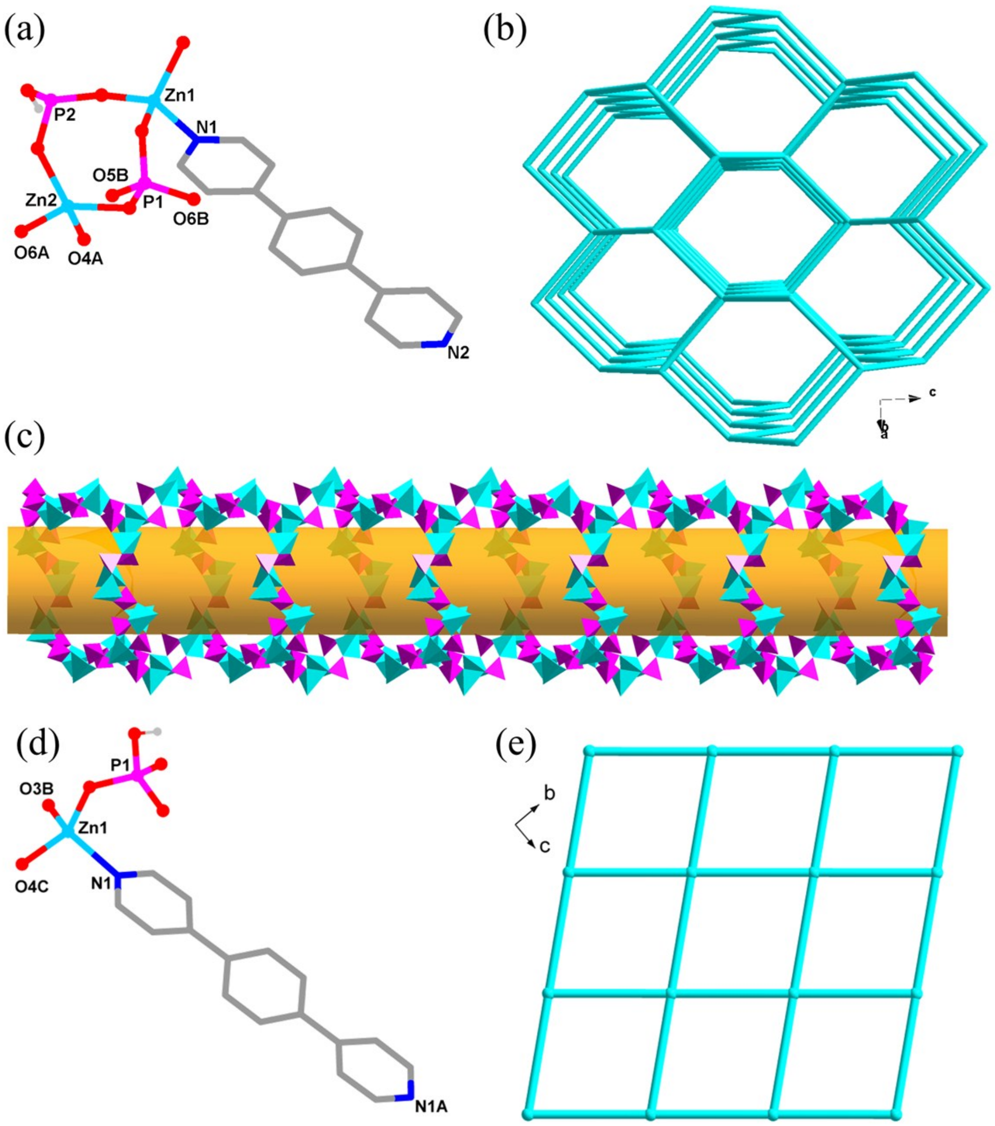

Fig. S1 (a) The coordination environments of Zn and P atoms (H atoms are omitted for clarity. Symmetry code: A) 1.25-*x*, *y*, 2.25-*z*. B) 1.25-*x*, 1.25-*y*, *z*.). (b) Topological view of the 3D framework of **1**. (c) Side view of the 20MR channel in **1**. (d) The coordination environments of Zn and P atoms (H atoms are omitted for clarity. Symmetry code: A) -*x*, -*y*, 1-*z*. B) 0.5-*x*, 0.5-*y*, 2-*z*. C) *x*, -*y*, 0.5+*z*.). (e) Topological view of the layer of **2**.

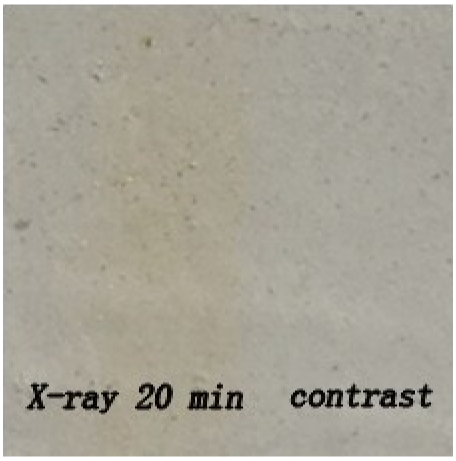

Fig. S2 The X-ray-induced color change for **1** (the former was captured using a powder X-ray diffractometer (Cu-K*a*, λ = 1.54187 Å; powered at 3 kW)).

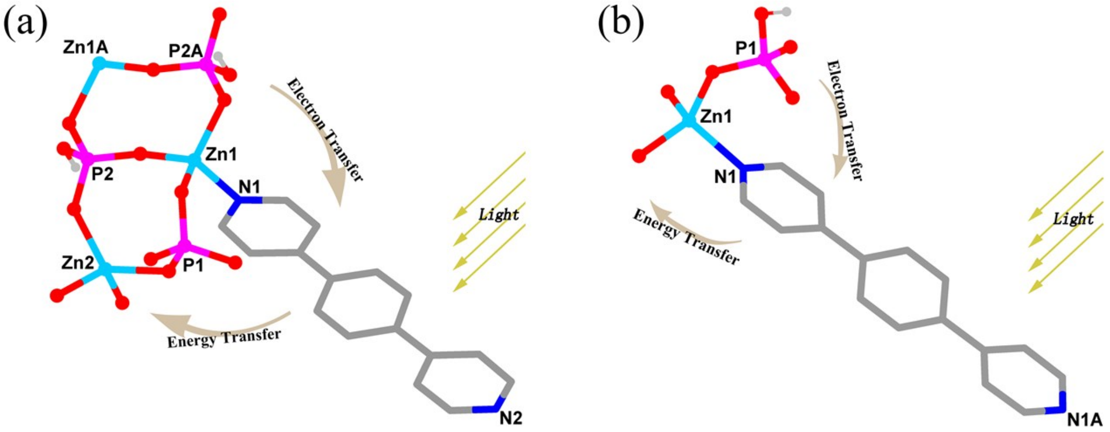

Fig. S3 The proposed photochromic mechanism of **1** (a) and **2** (b).

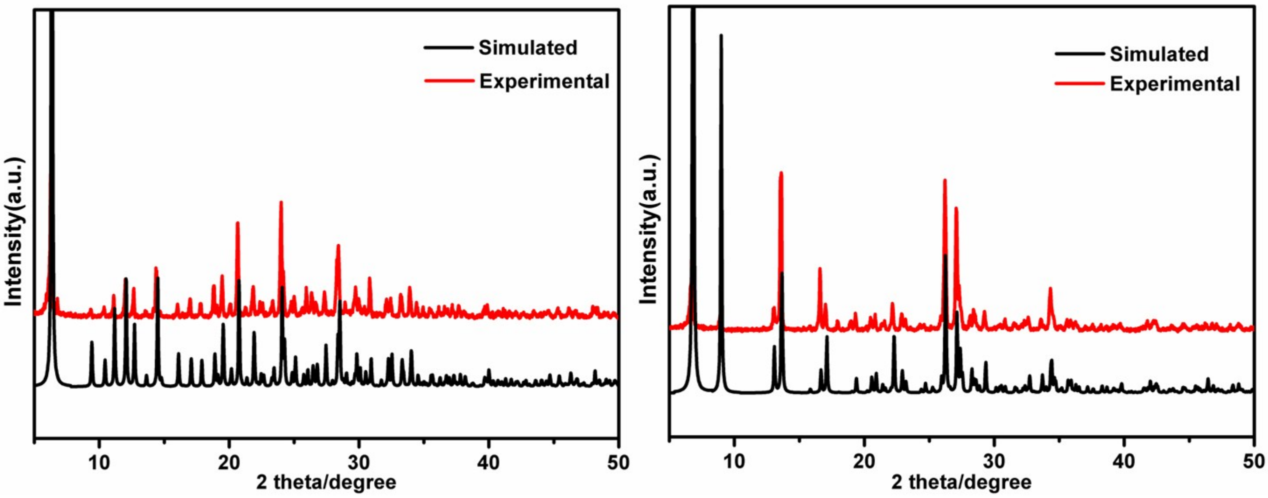

Fig. S4 PXRD patterns of **1** (left) and **2** (right).

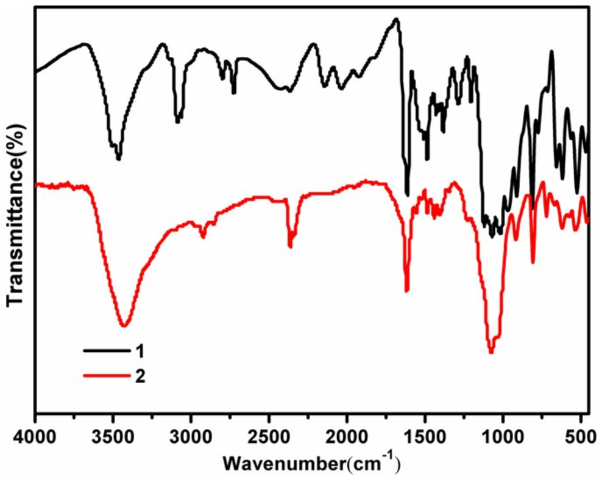

Fig. S5 The IR plots of **1** and **2**.

References

1. J. Seo, C. Bonneau, R. Matsuda, M. Takata and S. Kitagawa, *J. Am. Chem. Soc.*, 2011, **133**, 9005-9013.
2. G. Sheldrick, *Acta Crystallogr., Sect. C: Struct. Chem.*, 2015, **71**, 3–8.