Supporting Information

A stimuli-responsive zinc-based chain framework constructed via metal-ligand directed assembly

Mengchan Fan, Zhenguo Yao, Chen Li, Yu Xia, Qi Zhang, Jingcao Dai, Zhiyong Fu*

Experimental Section

All the reagents were purchased from commercial channels and used without further purification; N-(3-cyanophenyl)-4,4'-bipyridinium was synthesized as reported.[S1] UV-Visible spectral measurements were carried out using a HITACHI U-3010 spectrometer. The ESR spectrum was recorded at room temperature with a Bruker EMX-10/12 Electron Spin Resonance Spectrometer. IR spectrum was characterized by a Bruker Tensor 27 FTIR spectrometer in the range of 4000-400 cm^{-1} using a KBr disk. The C, H and N microanalyses were carried out with a Vario EL III elemental analyzer.

Synthesis of **1**: $Zn(NO_3)_2 \cdot 6H_2O$ (119.0 mg， 0.4mmol) was added to a mixture of benzenetetracarboxylic acid (50.8 mg，0.2 mmol), N-(3-cyanophenyl)-4,4'-bipyridinium chloride (51.6 mg, 0.2 mmol) in H_2O (0.5 ml), C_2H_5OH (1ml) and DMF (4ml). The mixture was stirred at room temperature for 15 min. Yellow block-like crystals were grown from the solution after a week. They were collected by filtration, washed by water and ethanol, and dried at room temperature (0.13 mmol, 63.6 mg, 65% yield based on N-(3-cyanophenyl)-4,4'-bipyridinium chloride). IR (KBr): v= 3550 (s), 3462 (s), 3122 (m), 3051 (m), 2237 (m), 1616 (s), 1577 (s), 1488 (s), 1427 (s), 1373 (s), 1143 (m), 1080 (w), 873 (m), 823 (s), 682 (m), 607 (s), 514 (m), 468 (w) cm^{-1}. Elemental analysis calcd (%) for $C_{22}H_{15}ClN_3O_5Zn$ (502.19): C, 52.62; H, 3.01; N, 8.37. found: C, 52.47; H, 2.94; N, 8.36.

References:

S1 D. Bongard, M. Möller, S. N. Rao, D. Corr and L. Walder, *Helv. Chim. Acta*, 2005, **88**, 3200.

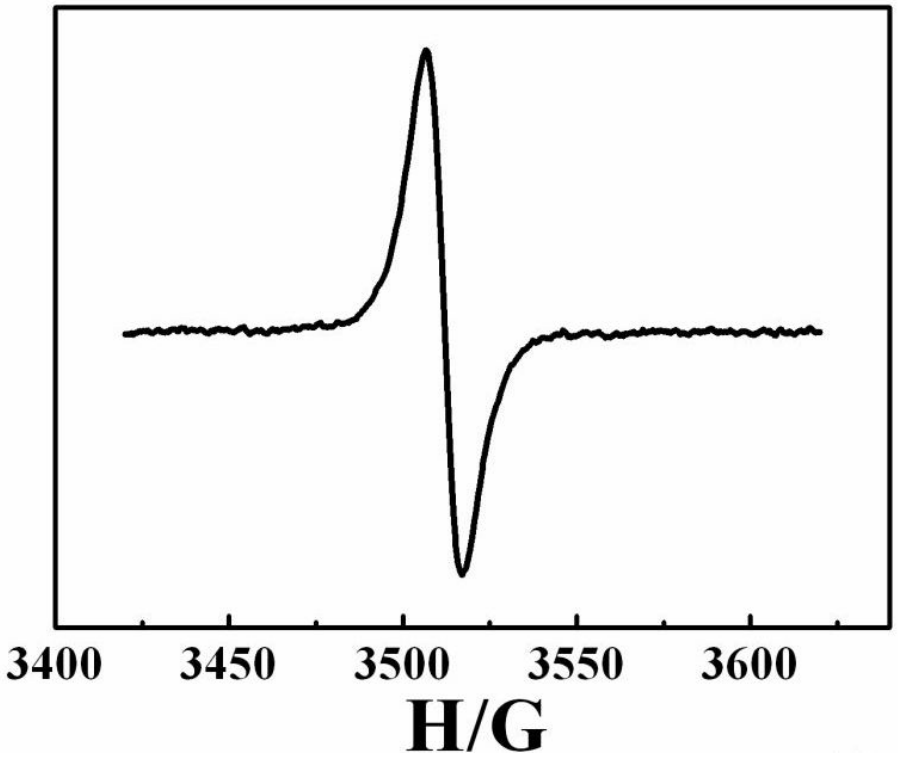

Fig. S1 ESR spectrum of compound **1.**

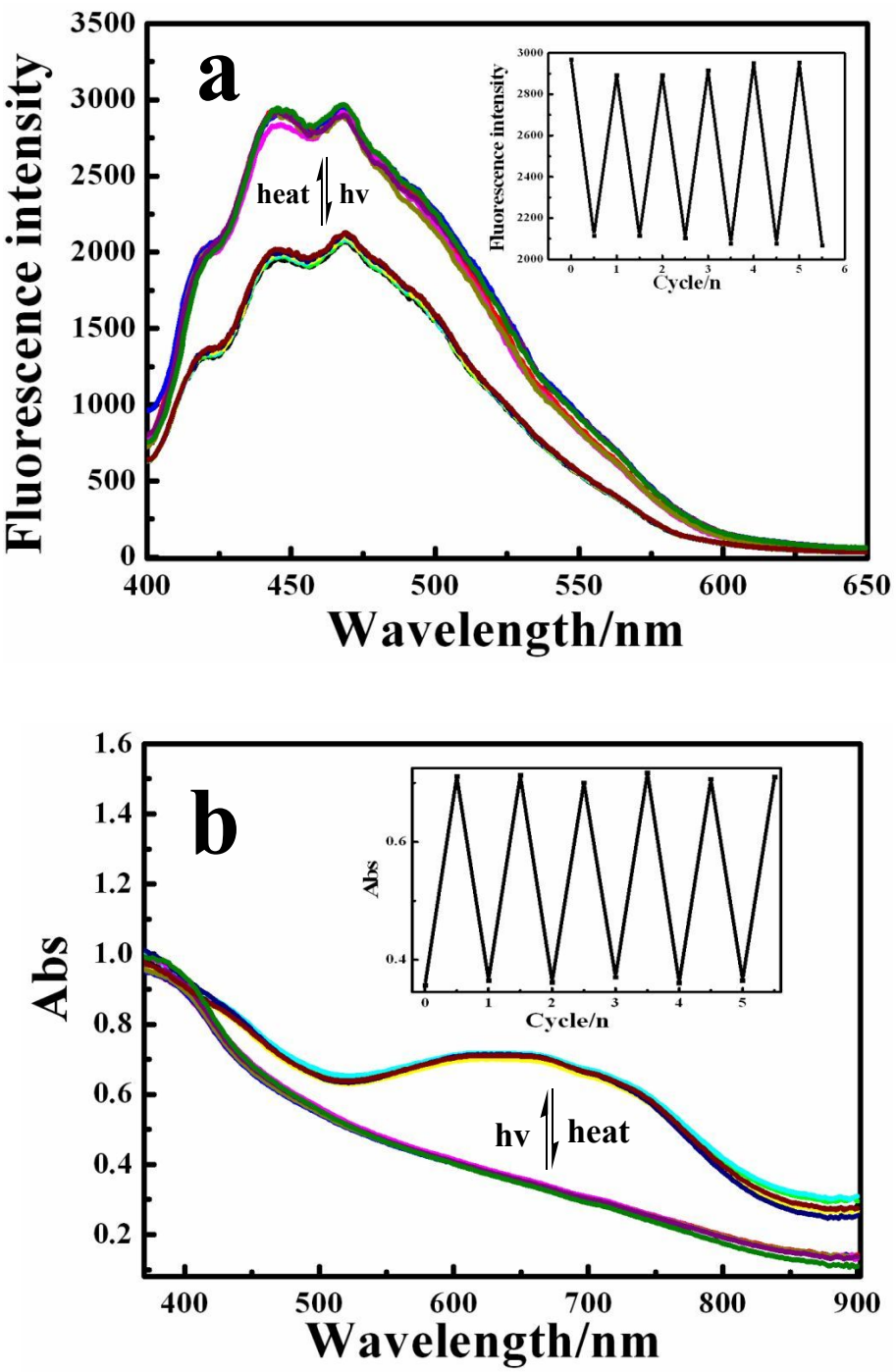

Fig. S2 Fluorescent emission changes at 450 nm (a) and UV-Vis absorbance changes at 665 nm (b) for the sample of **1** on alternate excitation by light irradiation and heated at 180°C over five cycles in air.

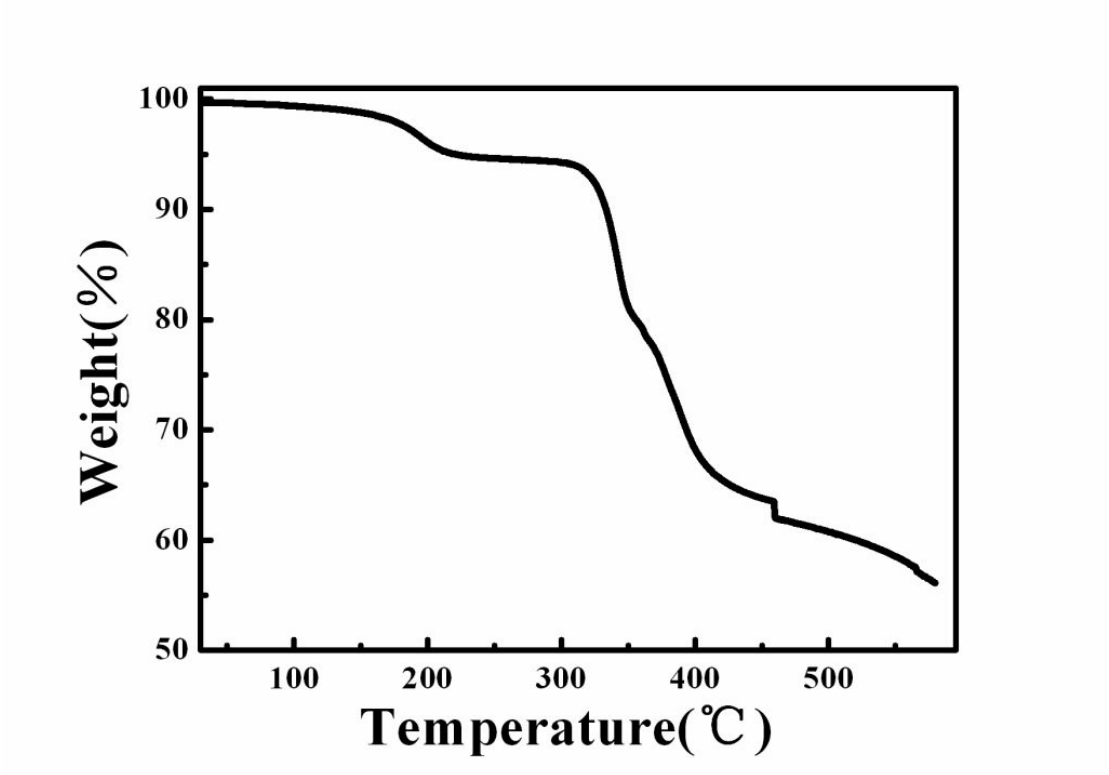

Fig. S3 Thermal gravimetric curve of **1**

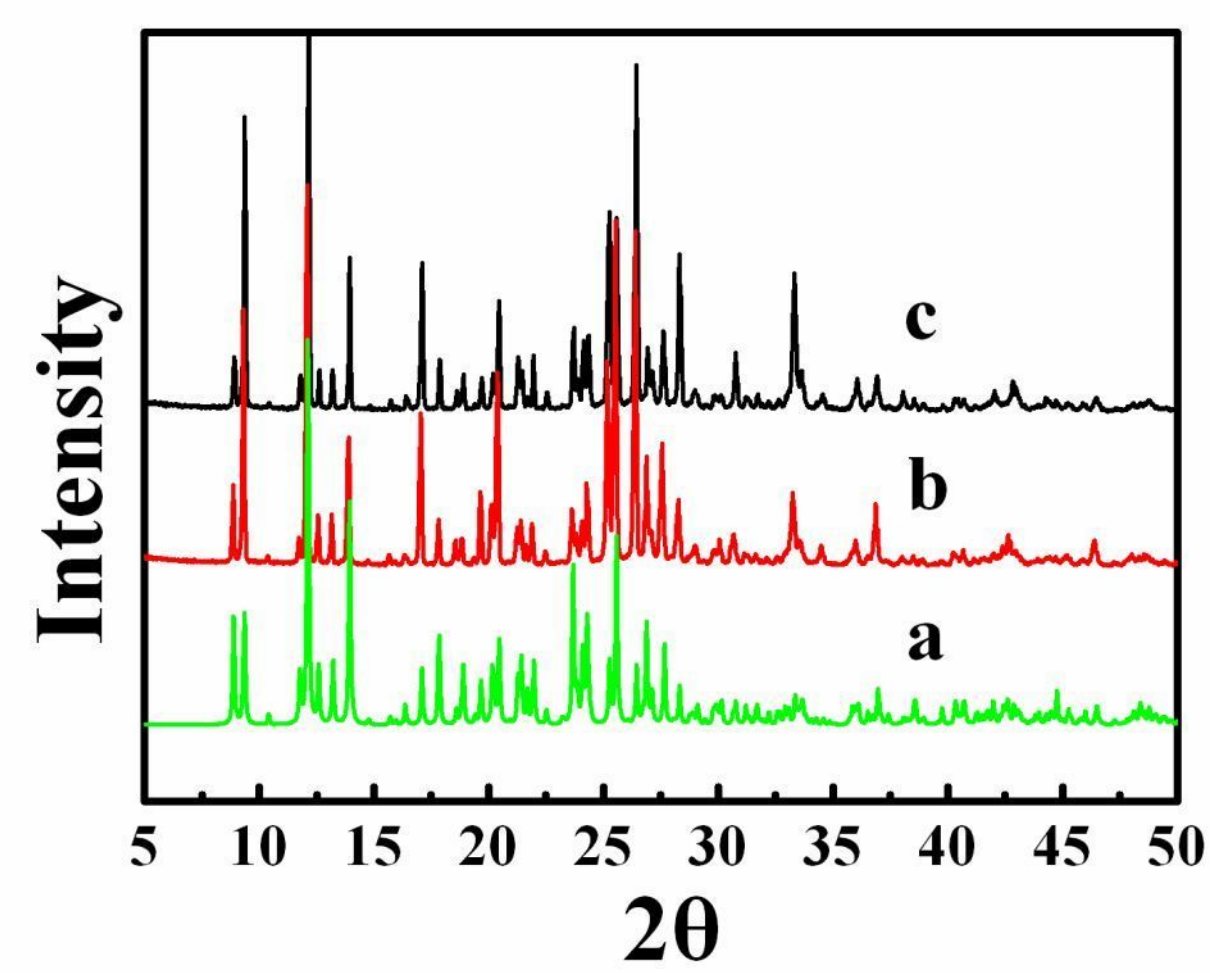

Fig. S4 Powder XRD patterns of **1 :** (a) simulated; (b) sample before light irradiation (yellow crystals); (c) sample after light irradiation (blue crystals).

Note: Phase purity of the bulk sample is confirmed by comparison of the simulated and observed XRD patterns. The same XRD patterns indicate that the structure of **1** does not change among the photochromic process.

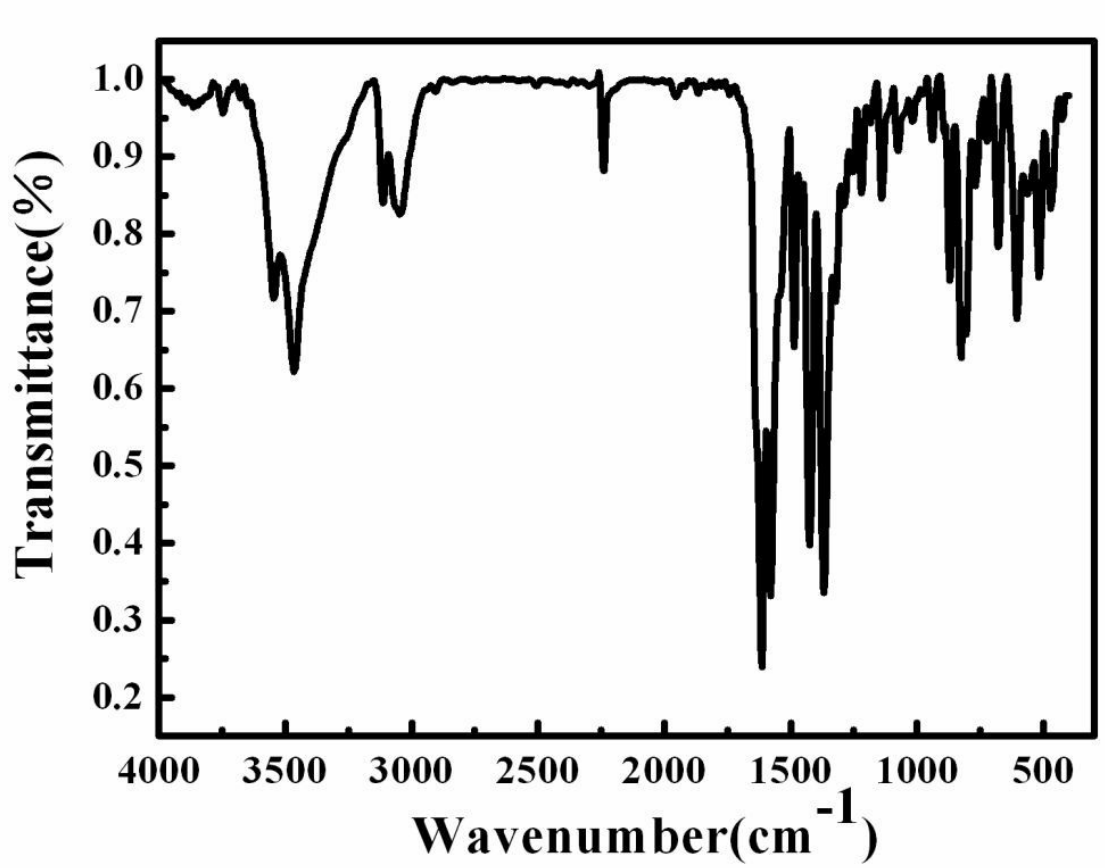

Fig. S5 IR spectrum of **1**