Supporting Information

Structure of a Cd(II) mixed-ligand coordination polymer: single crystalline conductance switch involving photoinduced electron transfer and photocoloration

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General methods and materials

All of the reagents were purchased from commercial channels and used without further purification; 4'-(4-pyridyl)-2,2':6',2''-terpyridine (PYTPY) was synthesized according to a reported method.[S1] A TA Instrument Q600 SDT thermogravimetric analyser was used to obtain the thermogravimetric analysis (TGA) curve in N_2 100 ml·min^{-1} at a rate of 10 °C·min^{-1}. The X-ray powder diffraction (XRD) data were collected in the angular range of 2θ = 5°-50° with a Bruker D8 Advance X-ray diffractometer using CuKα radiation (λ = 1.5406 Å). UV-Vis diffuse reflectance spectral measurements were carried out using a HITACHI U-3010 spectrometer, and a $BaSO_4$ plate was used as a 100% reflectance standard. Photoluminescence spectra were obtained using a F-7000 FL Spectrophotometer. The excitation wavelength used for emission spectra is 355 nm and the excitation/emission slit width were set to 5/5 nm. IR spectra were characterized by a Bruker Tensor 27 FTIR spectrometer in the range of 4000-400 cm^{-1} using KBr pellets. Electron spin resonance (ESR) signals were recorded at room temperature with a Bruker A300 Electron Spin Resonance Spectrometer. The C, H, N and S elemental analyses (EA) were performed on a Vario EL Ⅲ elemental analyzer. Temperature-dependent electrical conductivities and *I-V* curves were measured by a sourcemeter (Keithley Instrutments model 2636B).

[S1] L. Hou, D. Li, W. J. Shi, Y. G. Yin, S. W. Ng, *Inorg. Chem.* 2005, **44**, 7825.

Synthesis of compound 1

A mixture of $CdCl_2 \cdot 2.5H_2O$ (0.0114g, 0.05mmol), PYTPY (0.0080g, 0.0258mmol), H_2TDC (0.0129g, 0.075mmol) and H_2O (10mL)was stirred for 30 min in air, and then transferred and sealed in a 25mL Teflon-lined steel bomb, which was heated at 160°C for 48 h and then cooled to room temperature at a rate of 5 °C h^{-1}. Finally, pale yellow crystals were collected by filtration, washed with DMF and distilled water for 3 times and then dried at room temperature for 12 h (0.0030g, 37.50% based on PYTPY). IR data: 3516(w), 3078(m), 1587(s), 1531 (s), 1362(vs), 1233(m), 1151(m), 1007(m), 812(m), 783(m), 622(m), 488(m). Anal. Calc. (%) for **1**: C 52.67, H 2.72, N 9.45, S 5.41; found: C 52.56, H 2.74, N 9.50, S 5.45.

X-ray single crystal diffraction

The data were measured on a Agilent Gemini E diffractometer with graphite monochromated Mo/Kα radiation (λ = 0.71073 Å). Data were collected at 293K, using the ω- and φ-scans to a maximum θ value of 25.02°. Absorption corrections were performed using a multi-scan method. The structures were solved by direct methods with SHELXS-97 and refined by full-matrix least-square technique on F^2 with SHELXL-97. Non-hydrogen atoms were all refined anisotropically. Hydrogen atoms were included at geometrically idealized positions and thermal parameters were fixed during structural refinement. CCDC 1855102 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.ukf/data_request/cif.

Table S1. Crystal data for 1.

Empirical formula	$C_{26}H_{16}CdN_4O_4S$	
Formula weight	592.89 g/mol	
Crystal system	Triclinic	
Space group	*P -1*	
Unit cell dimensions	a = 8.7461(3) Å	α = 83.381(4)°
	b = 10.7477(5) Å	*β* = 75.005(4)°
	c = 13.2654(6) Å	γ = 69.554(4)°
Volume	1128.18(10) $Å^3$	
Crystal density (calculated)	1.745 g/cm^3	
F (000)	592	
Goodness-of-fit on F^2	1.081	
Final *R* indices [I >2σ (I)]	R_1 = 0.0486, ${}_wR_2$ = 0.1062	
R indices [all data]	R_1 = 0.0520, ${}_wR_2$ = 0.1079	

[a] $R_1 = \sum || F_o| - |F_c|| / \sum |F_o|$. $wR_2 = [\sum [w (F2\ o - F2\ c)^2] / \sum [w (F2\ o)^2]]^{1/2}$.

PXRD Analysis

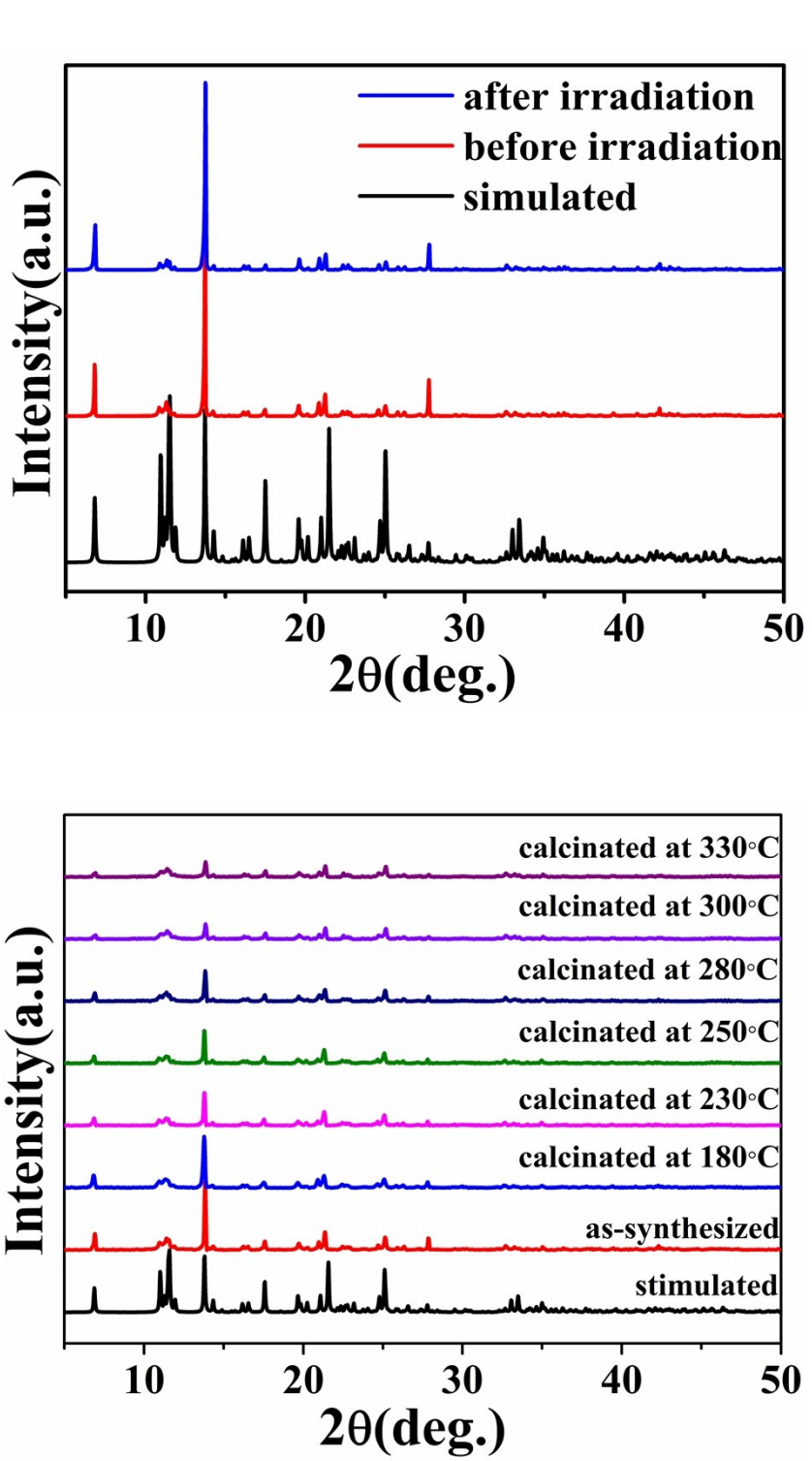

Fig. S1 (a) Simulated and experimental powder X-ray diffraction patterns of **1**; (b) Powder XRD patterns of samples calcined at different temperatures.

UV-vis spectrum

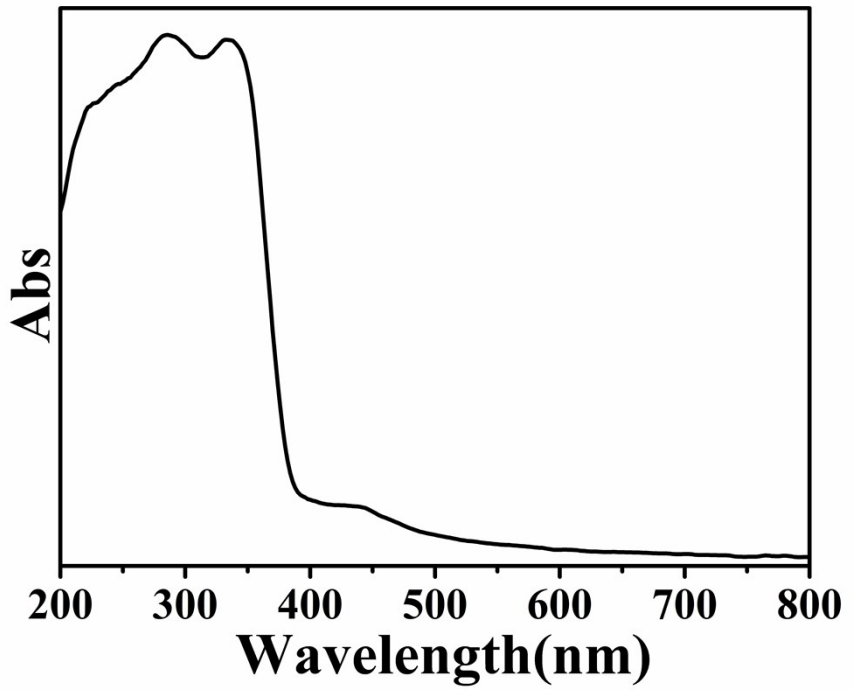

Fig. S2 UV-vis spectrum of compound **1**.

ESR analysis

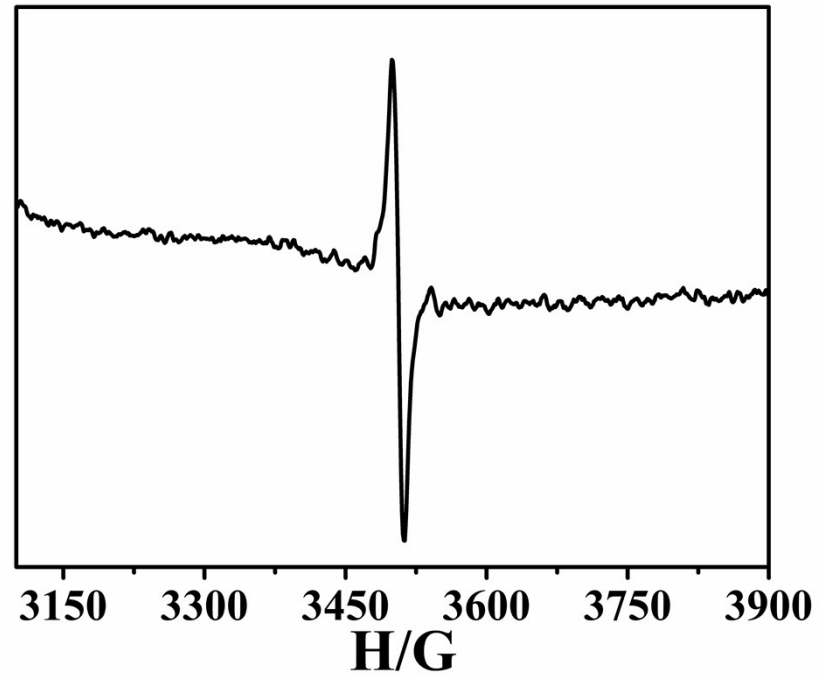

Fig. S3 ESR spectrum of **1** after photoirradiation.

TG Analysis

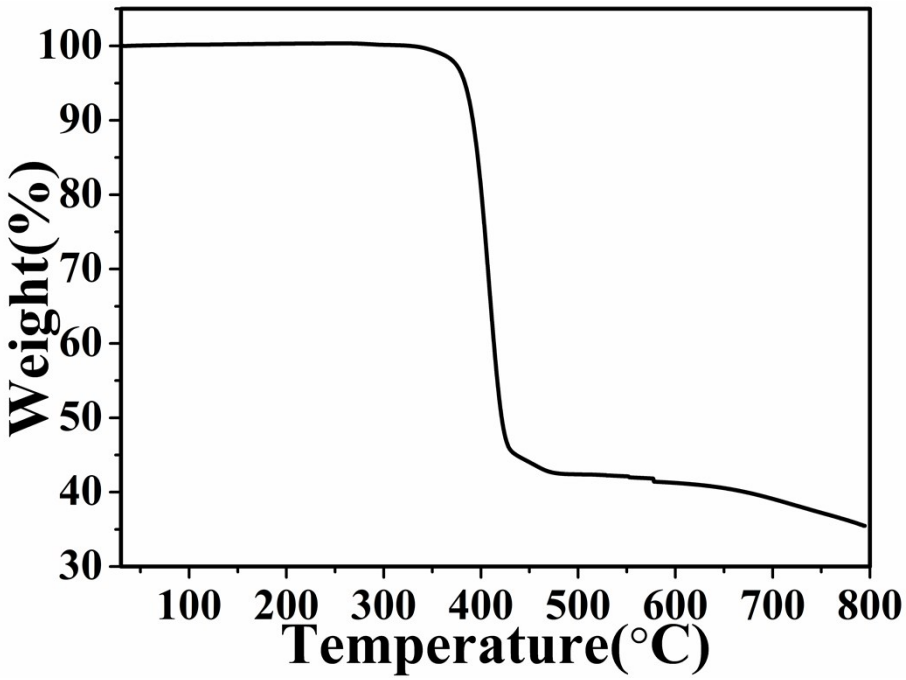

Fig. S4 Thermal gravimetric curve of compound **1**.

Thermal conductivity analysis

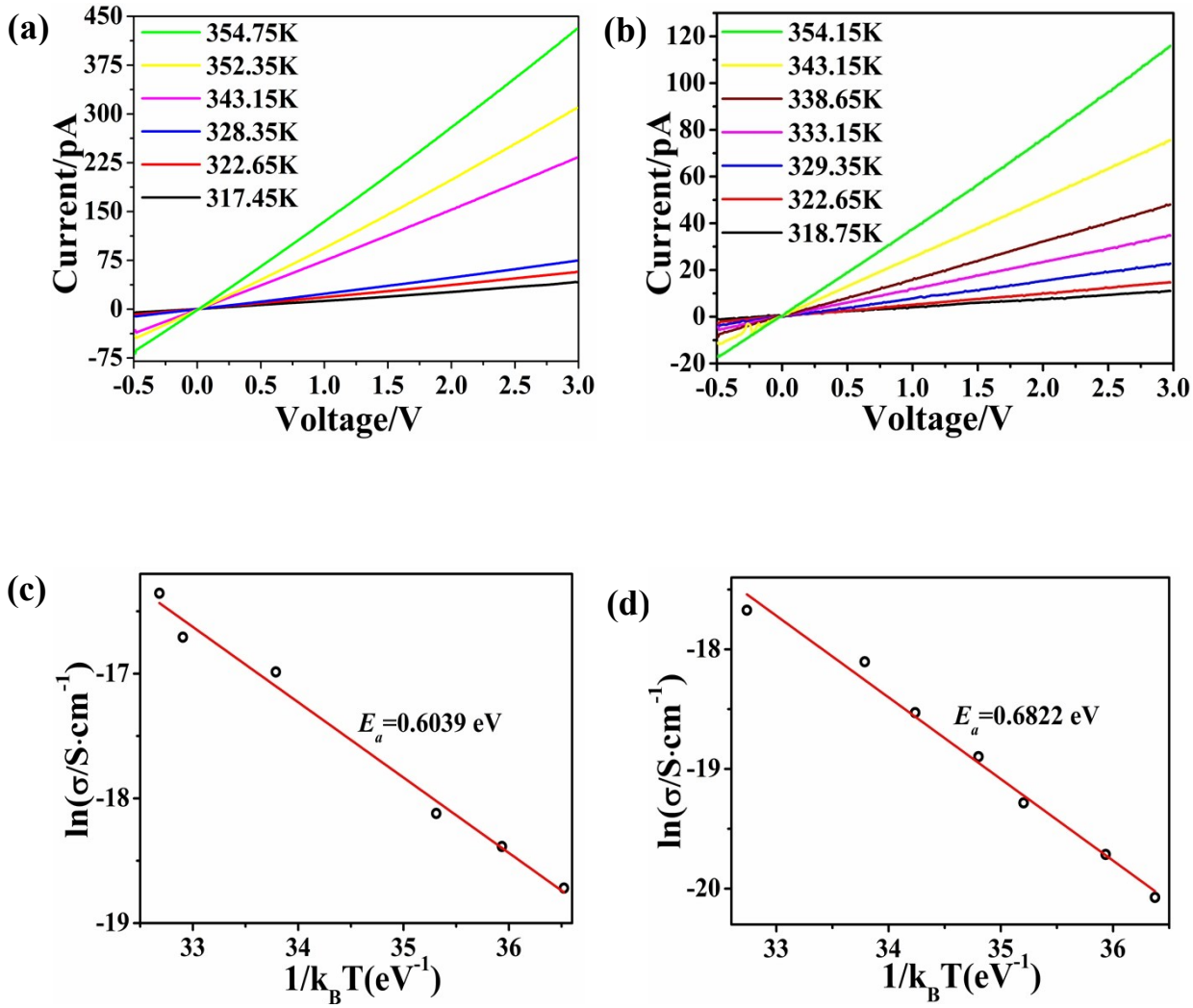

Fig. S5 Temperature-dependent *I–V* curves before irradiation (a) and after irradiation (b). Arrhenius plots before irradiation (c) and after irradiation (d). E_a is the activation energy.

IR spectrum

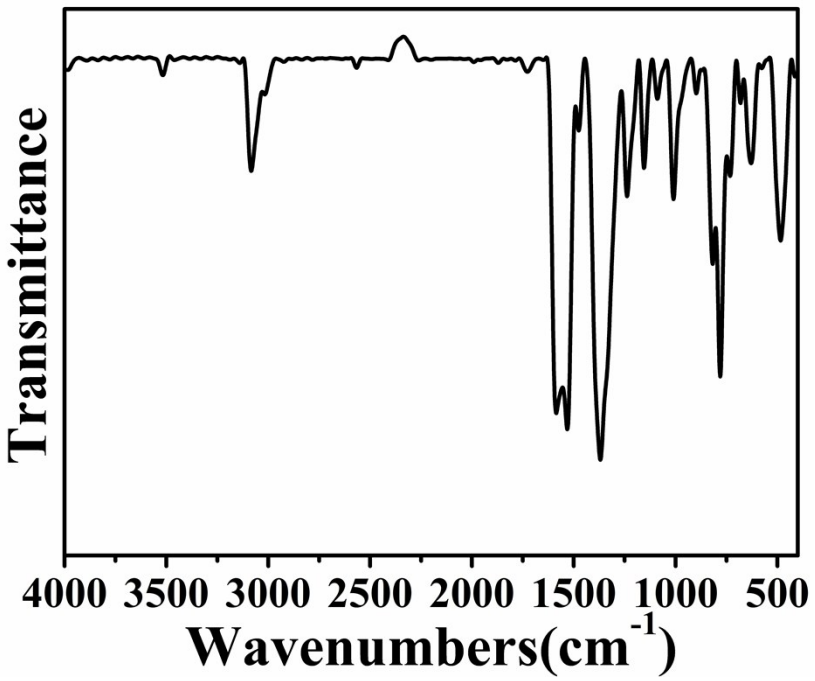

Fig. S6 IR spectrum of **1**.