Supporting Information (SI)

The modulation effect of auxiliary ligands on photochromic properties of 3D naphthalene diimide coordination polymers

Shimin Zhang, Weiyu Yu, Pengfei Hao,* Gaopeng Li, Junju Shen and Yunlong Fu*

Key Laboratory of Magnetic Molecules & Magnetic Information Materials Ministry of Education, School of Chemical and Material Science, Shanxi Normal University, Taiyuan 030031, China

E- mail: haopengfei_2015@126.com; yunlongfu@sxnu.edu.cn

Content

1.Figures

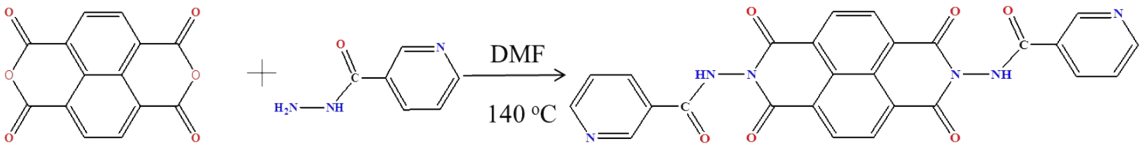

Fig. S1 The Chem Draw type diagram of NicNDI ligands (NicNDI = (3-pyridylacylamino)-1,4,5,8-naphthalene diimide)

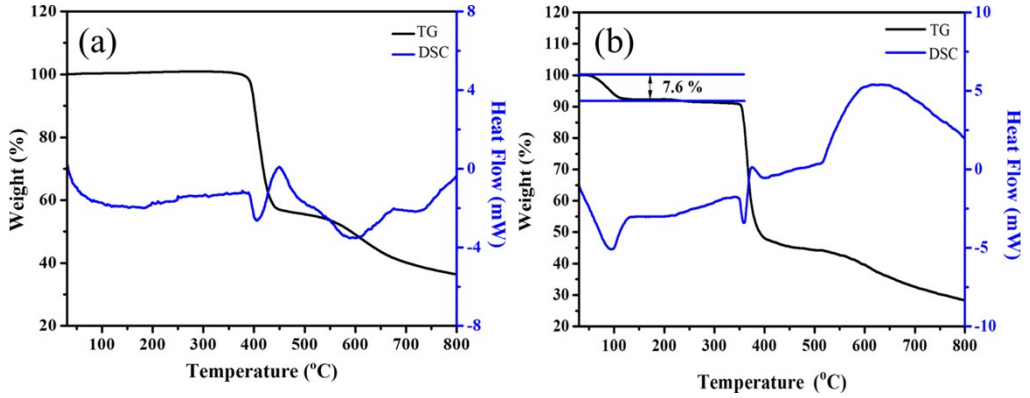

Fig. S2 TGA curve of **1** (a) and **2** (b).

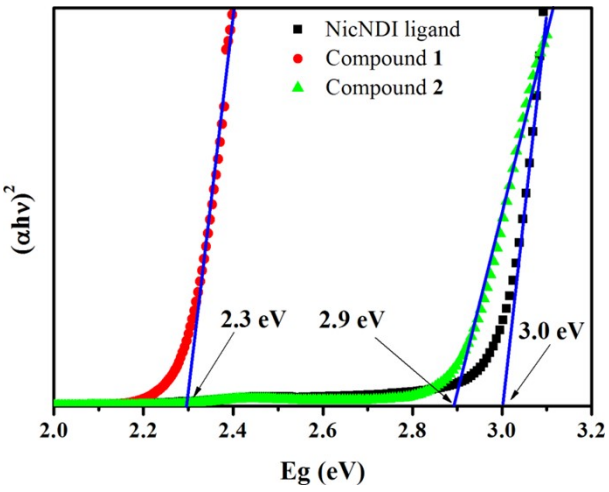

Fig. S3 The optical band gaps of NicNDI ligand (black), **1** (red) and **2** (green)

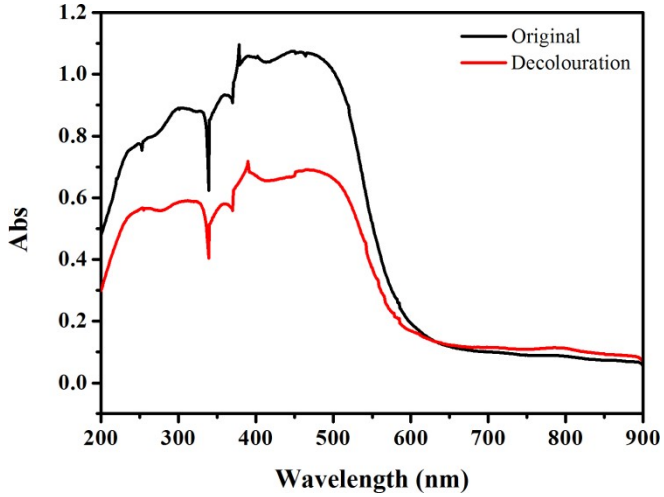

Fig. S4 The UV-vis absorption spectra of the original sample and decolourations sample of **1**.

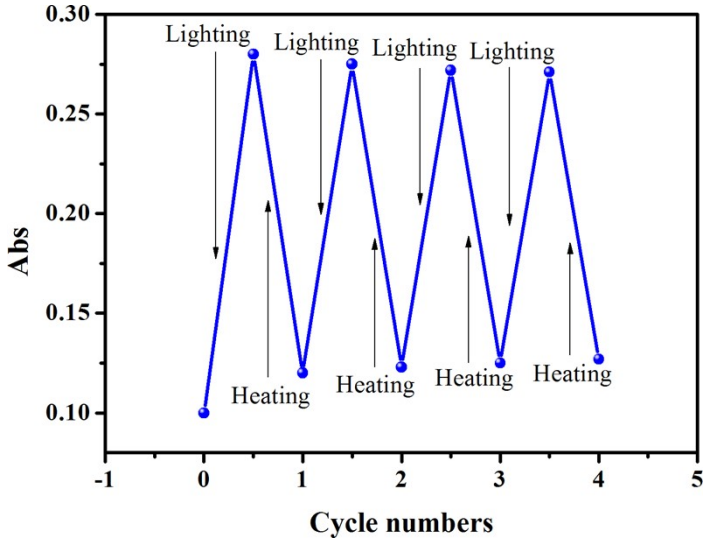

Fig. S5 The coloration-decoloration processes with repeated UV irradiation/heating of **1**.

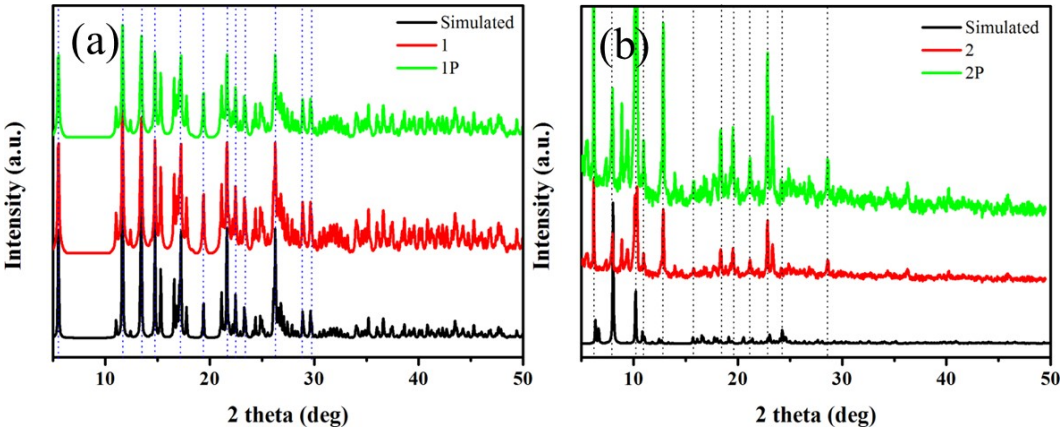

Fig. S6 Powder X-ray diffraction (PXRD) patterns of **1**, **1P**, **2** and **2P** at room temperature.

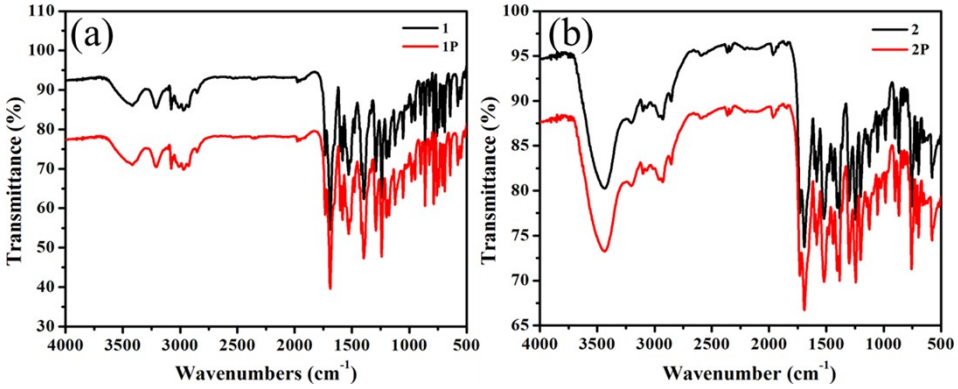

Fig. S7 IR spectra of **1**, **1P**, **2** and **2P**.

2. Tables

Table S1 Crystallographic data and refinement parameters of **1** and **2**.

Compound	**1**	**2**
Empirical formula	$C_{42}H_{24}CdN_6O_{10}$	$C_{40}H_{22}CdN_6O_{10}$
Formula weight	885.07	859.03
Temperature (K)	293(2)	293(2)
Crystal system	monoclinic	monoclinic
Space group	*C*2/*c*	*C*2/*c*
a (Å)	34.294(2)	17.3232(19)
b (Å)	7.2986(6)	28.428(3)
c (Å)	15.2539(13)	18.805(3)
α (°)	90	90
β (°)	110.932(2)	112.765(3)
γ (°)	90	90
V (Å^3)	3566.1(5)	8539.4(19)
Z	4	8
D_c (g cm^{-3})	1.649	1.336
μ (mm^{-1})	0.687	0.571
F(000)	1784.0	3456.0
Crystal size/mm^3	0.846 × 0.246 × 0.173	0.137 × 0.108 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
ϑ range (°)	5.724 to 56.714	4.326 to 56.836
Reflections collected	25587	63082
Unique reflections	4465	10679
R_{int}	0.0769	0.0896
Data/restraints/parameters	4465/0/267	10679/0/514
Goodness-of-fit on F^2	1.055	1.046
R_1/wR_2, $[I \geq 2\sigma(I)]^{a,b}$	0.0485/0.0996	0.0792/0.2374
R_1/wR_2, (all data)	0.0873/0.1121	0.1399/0.2693
$\Delta\rho_{max}/\Delta\rho_{min}$ (e Å^{-3})	1.33/-0.58	1.97/-1.00

Table S2 Selected bond lengths (Å) and angles (°) of **1** and **2**.

Compound **1**			
Cd1-N1[1]	2.305(3)	Cd1-O1[1]	2.376(2)
Cd1-N1	2.305(3)	Cd1-O1	2.376(2)
Cd1-O2	2.281(2)	Cd1-O2[1]	2.281(2)
N1[1]-Cd1-N1	87.36(13)	O2[1]-Cd1-N1[1]	143.57(9)
N1[1]-Cd1-O1[1]	93.07(8)	O2[1]-Cd1-N1	91.13(9)
N1[1]-Cd1-O1	118.38(8)	O2[1]-Cd1-O1	98.05(8)
N1-Cd1-O1	93.07(8)	O2-Cd1-O1	56.17(8)
N1-Cd1-O1[1]	118.37(8)	O2[1]-Cd1-O1[1]	56.17(8)
O1[1]-Cd1-O1	137.11(11)	O2-Cd1-O1[1]	98.05(8)
O2-Cd1-N1[1]	91.13(9)	O2-Cd1-O2[1]	110.51(13)
O2-Cd1-N1	143.58(9)		
symmetry codes: [1]-x,+y,1/2-z; [2]-x,1-y,1-z; [3]1/2-x,-1/2-y,1-z			

Compound **2**			
Cd1-O1	2.266(5)	Cd1-O7	2.455(4)
Cd1-O9[1]	2.263(4)	Cd1-O10[1]	2.444(4)
Cd1-N1	2.297(4)	Cd1-N2	2.317(4)
O1-Cd1-O7	54.97(14)	O1-Cd1-O10[1]	99.74(15)
O1-Cd1-N1	137.24(16)	O1-Cd1-N2	88.66(17)
O9[1]-Cd1-O1	112.25(18)	O91-Cd1-O7	104.14(16)
O9[1]-Cd1-N1	90.81(17)	O91-Cd1-O10[1]	55.13(14)
O9[1]-Cd1-N2	140.59(18)	O10[1]-Cd1-O7	141.55(14)
N1-Cd1-O7	85.43(15)	N1-Cd1-O10[1]	122.76(15)
N2-Cd1-O7	115.12(17)	N2-Cd1-O10[1]	89.68(16)
symmetry codes: [1]-x,+y,1/2-z; [2]-x,1-y,1-z; [3]1/2-x,-1/2-y,1-z			

Table S3 Hydrogen bonds of **1** and **2** (Å and °).

Compound **1**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N2-H2···O1[1]	0.86	2.09	2.909(4)	157.9
symmetry codes: [1]-x,+y,1/2-z; [2]-x,1-y,1-z; [3]1/2-x,-1/2-y,1-z				

Compound **2**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N3-H3···O10[1]	0.86	1.93	2.752(7)	158.5
N5-H5···O7[2]	0.86	1.99	2.807(7)	159.3
symmetry codes: [1]-x,+y,1/2-z; [2]-x,1-y,1-z; [3]1/2-x,-1/2-y,1-z				