Supporting Information (SI)

Ultrafast visible-light photochromic properties of naphthalenediimide-based coordination polymers for the visual detecting/filtering blue light

Pengfei Hao,* Bohong Gao, 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 address: haopengfei_2015@126.com; yunlongfu@sxnu.edu.cn.

Content

1. Figures

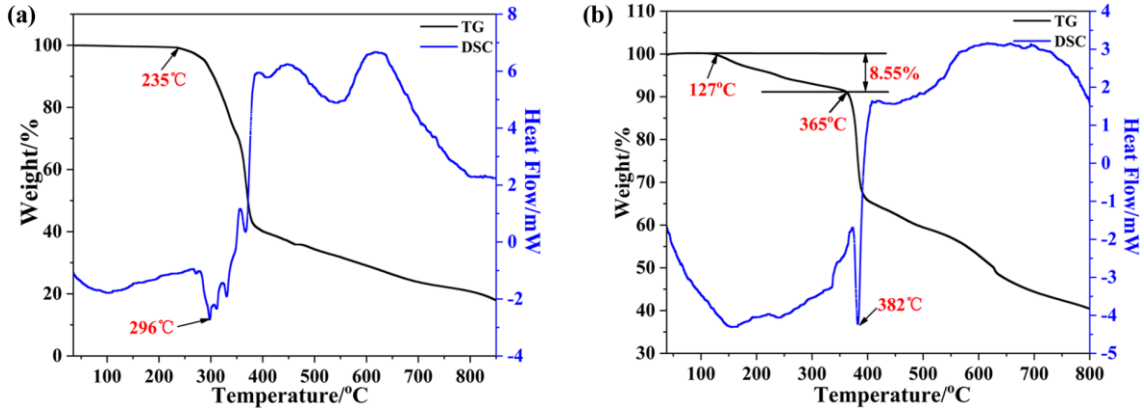

Fig. S1 Thermo-gravimetric (TG) and Differential scanning calorimetry (DSC) curves of **1** and **2**.

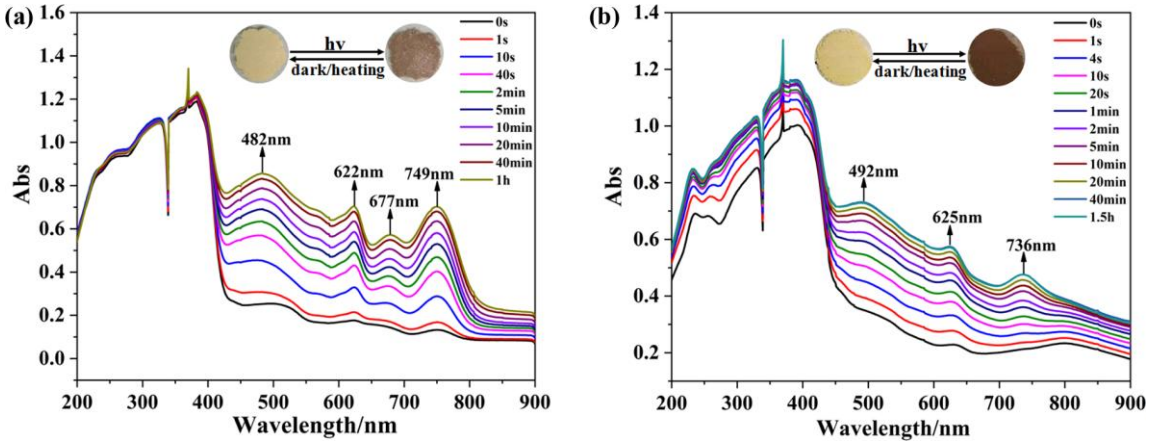

Fig. S2 The UV-vis absorption spectra of 3-/4-PMNDI upon alternating UV light illumination and dark/heat treatment.

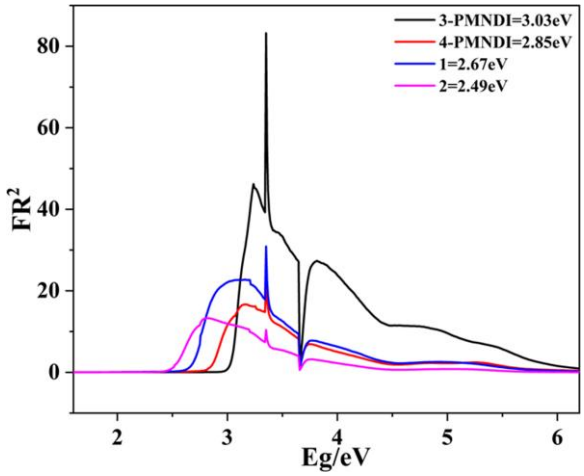

Fig. S3 Kubelka-Munk transformed reflectivity *vs* energy of complexes **1**, **2**, 3-PMNDI and 4-PMNDI.

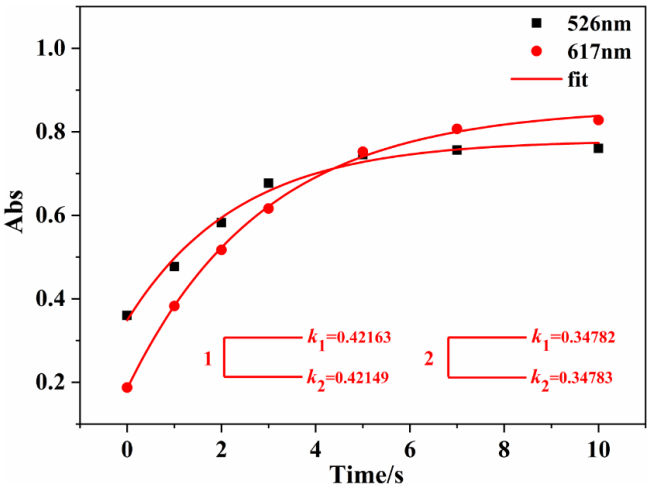

Fig. S4 Abs(*t*) *vs. t* plots for **1-2**. The lines show the fits of the plots according to rate law Abs(*t*) = A_0 + A_1(exp(-k_1t) + exp(-k_2t)) (*inset*: coloration rate constant values of **1-2**) (λ_{max} = 526 nm for **1** and λ_{max} = 617 nm for **2**).

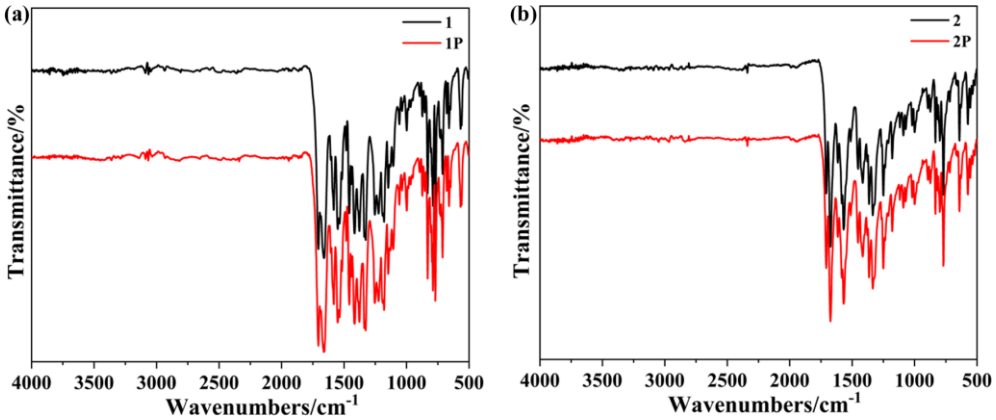

Fig. S5 FT-IR spectra of **1** and **2** as-synthesized samples and after irradiation samples.

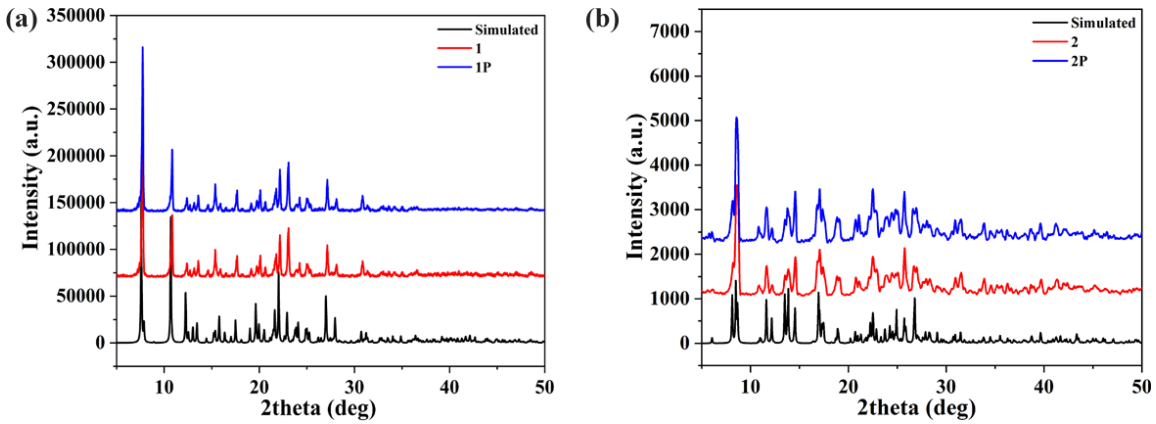

Fig. S6 PXRD patterns of **1** and **2** simulated from the X-ray single-crystal structures, as-synthesized samples and after irradiation samples.

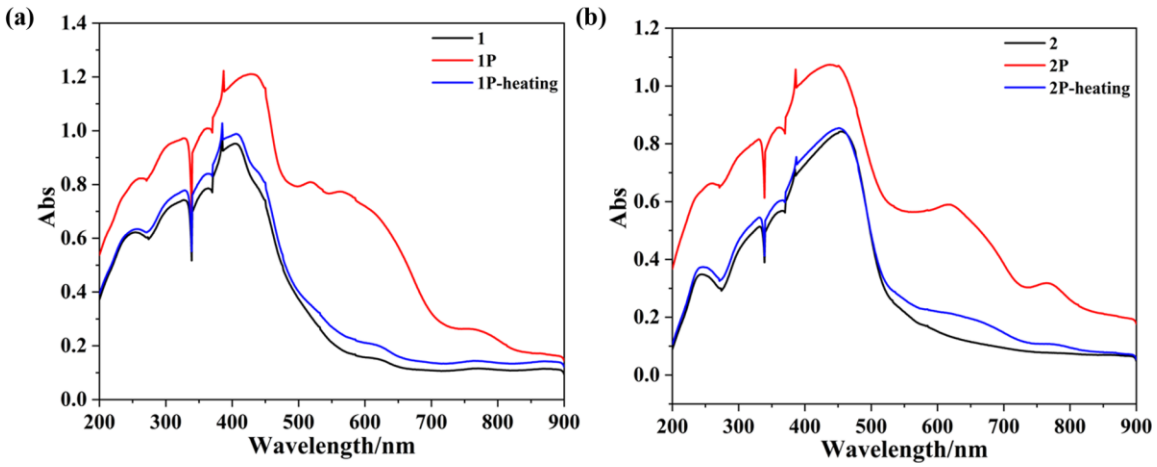

Fig. S7 The UV-vis absorption spectra of **1**, **1P** and **1P**-heating (a) and **2**, **2P** and **2P**-heating (b).

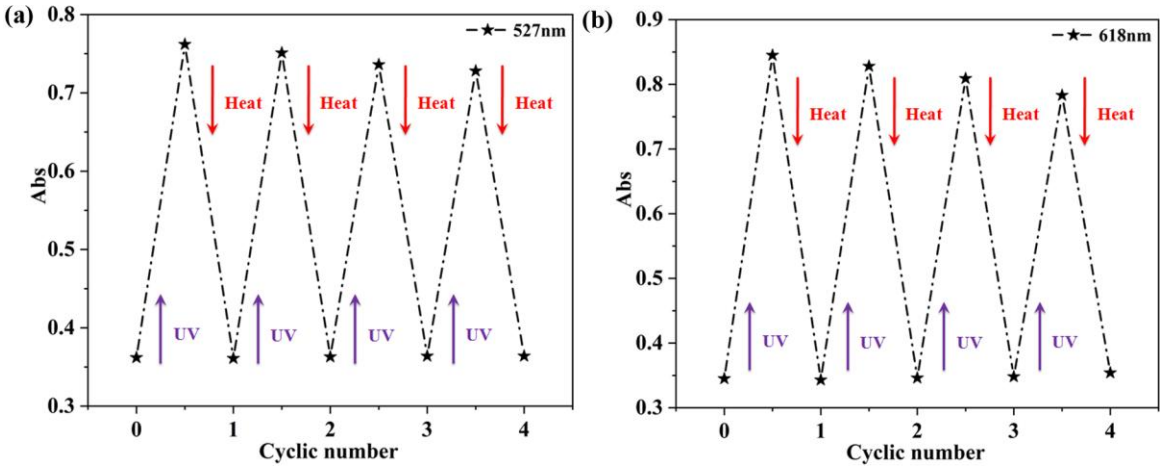

Fig. S8 The switching cycles of coloration-decoloration processes of **1** (527nm) and **2** (618nm) upon alternating Xe light illumination and thermal treatment.

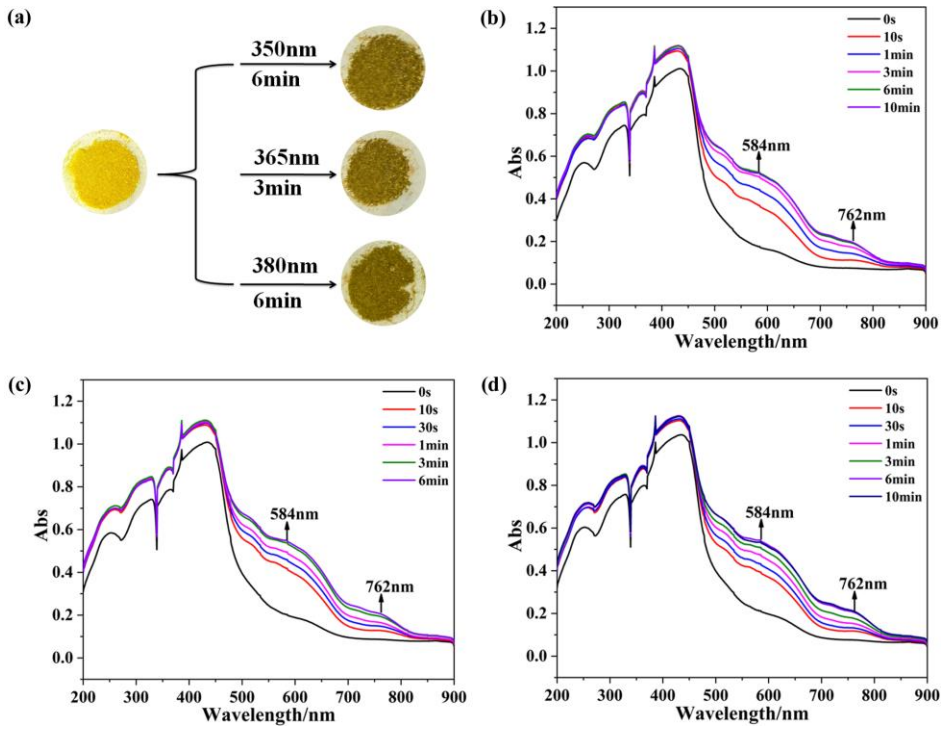

Fig. S9 The photochromic behaviors and UV-vis absorption spectra of **1** upon UV light (335-395 nm) illumination.

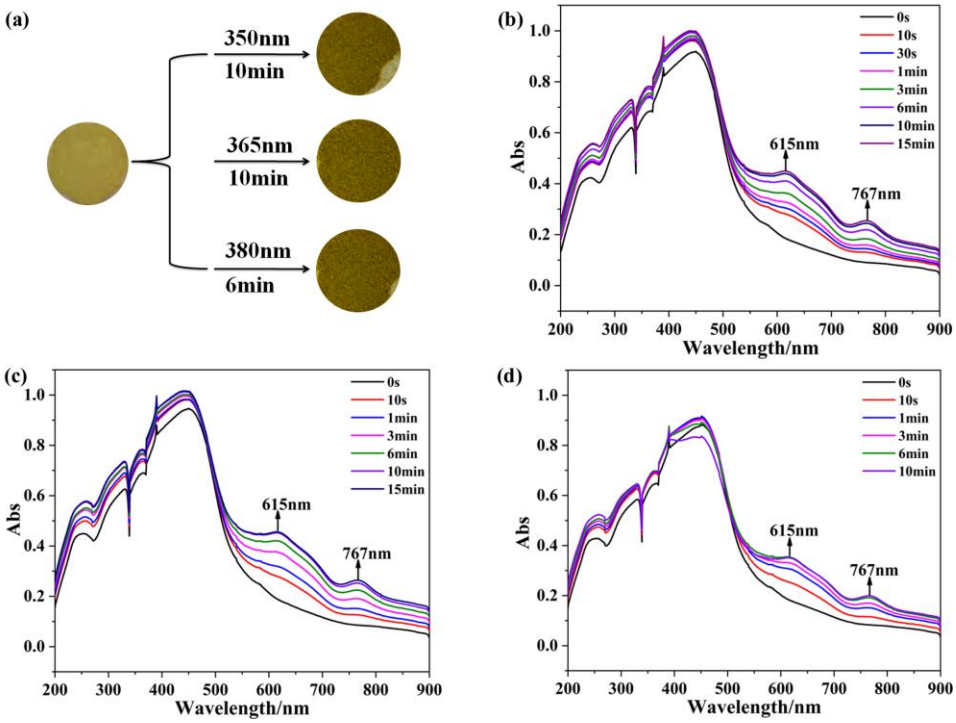

Fig. S10 The photochromic behaviors and UV-vis absorption spectra of **2** upon UV light (335-395 nm) illumination.

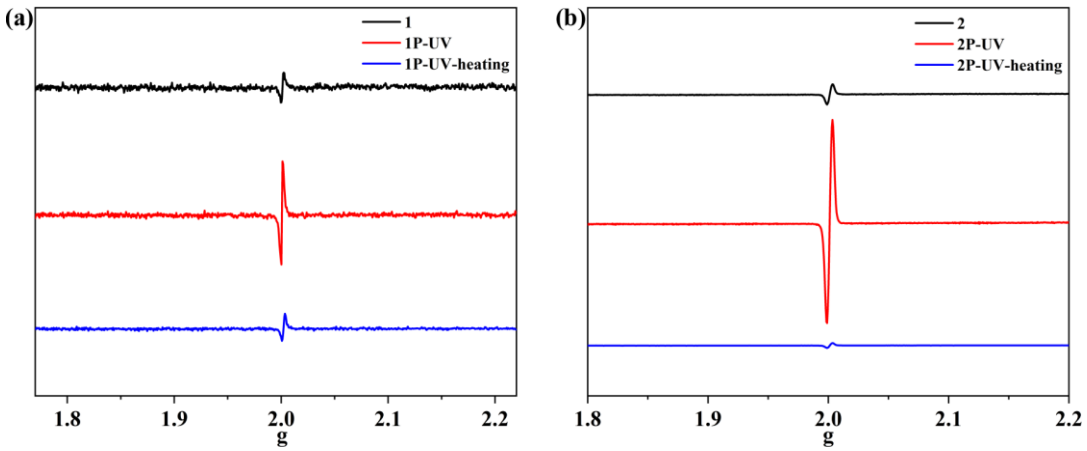

Fig. S11 The EPR spectra of **1**, **1P**-UV and **1P**-UV-heating (a), and **2**, **2P**-UV and **2P**-UV-heating (b).

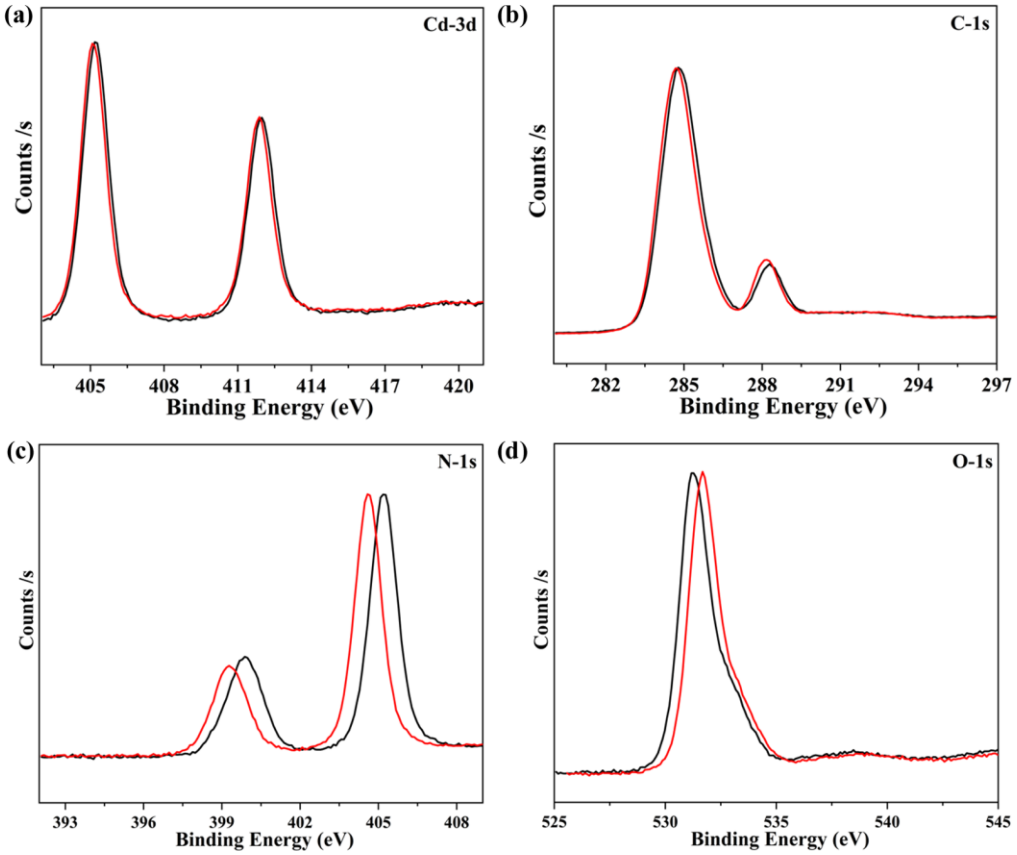

Fig. S12 Cd 3d (a), C 1s (b), N 1s (c) and O 1s (d) XPS core-level spectra of **1** and **1P**.

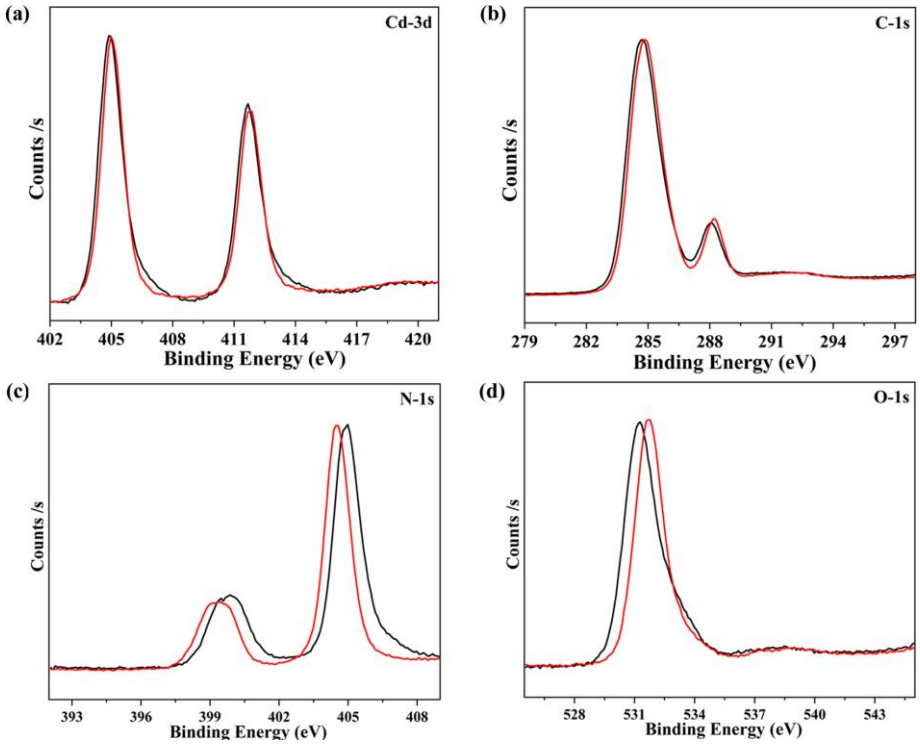

Fig. S13 Cd 3d (a), C 1s (b), N 1s (c) and O 1s (d) XPS core-level spectra of **2** and **2P**.

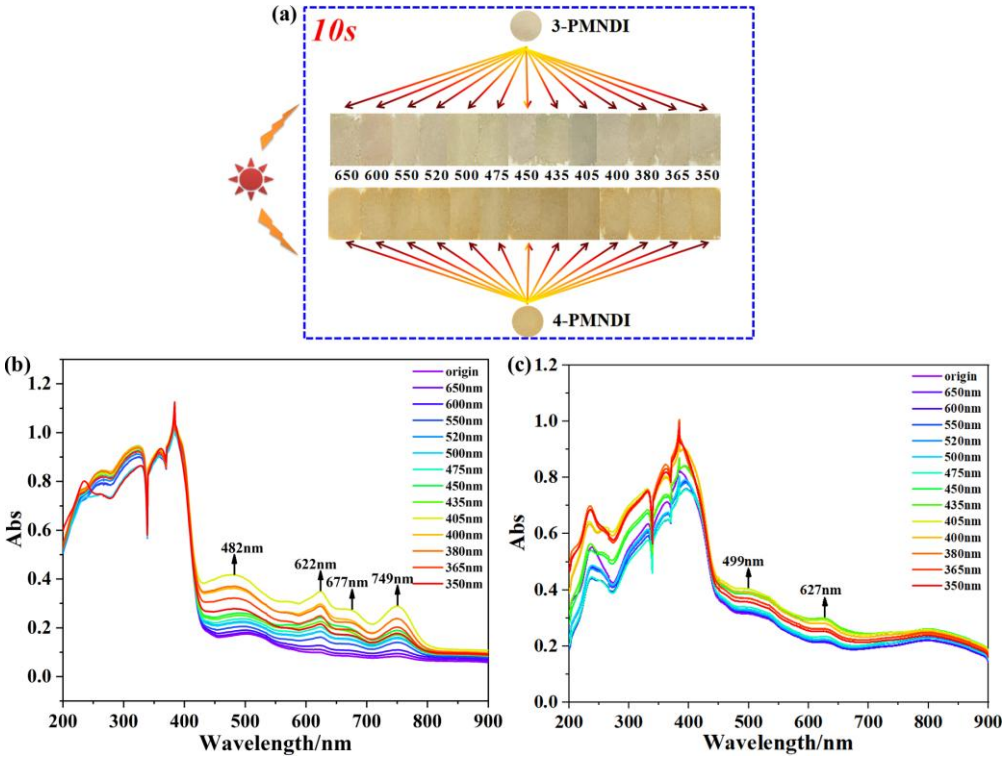

Fig. S14 The photochromic behaviors of 3-/4-PMNDI (a), and the UV-vis absorption spectra of 3-PMNDI (b) and 4-PMNDI (c) under excitation of different visible-light wavelengths.

2. Tables

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

Compounds	**1**	**2**
CCDC code	2110413	2110414
Empirical formula	$C_{52}H_{34}CdN_5O_{13}$	$C_{41}H_{22}CdN_5O_9$
Formula weight	1049.24	841.03
Temperature (K)	293(2)	293(2)
Crystal system	monoclinic	orthorhombic
Space group	I_2/a	*Pccn*
a (Å)	15.0583(10)	20.383(4)
b (Å)	13.6049(9)	20.776(4)
c (Å)	23.4146(15)	16.393(3)
α (°)	90	90
β (°)	106.508(4)	90
γ (°)	90	90
V (Å^3)	4599.1(5)	6942(2)
Z	4	8
D_c (g cm^{-3})	1.515	1.609
μ (mm^{-1})	0.550	0.698
F(000)	2132.0	3384.0
Crystal size(mm^3)	0.253 × 0.125 × 0.029	0.211 × 0.135 × 0.045
Θ range (°)	5.778 to 56.672	5.054 to 39.682
Reflections collected	33566	89401
R_{int}	0.0271	0.0480
Data/restraints/parameters	5724/20/336	3156/172/551
Goodness-of-fit on F^2	1.090	1.083
R_1/wR_2, [$I \geq 2\sigma(I)$][a,b]	0.0389/0.1099	0.0487/0.1299
R_1/wR_2, [$I \geq 2\sigma(I)$][a,b] [all data]	0.0480/0.1153	0.0549/0.1345

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

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

Compound **1**			
Cd(1)-O(7)	2.334(3)	C(4)-C(5)	1.385(4)
Cd(1)-O(3)	2.5583(19)	C(4)-C(6)	1.505(4)
Cd(1)-O(3)#1	2.5584(19)	C(7)-C(12)	1.479(4)
Cd(1)-O(4)	2.3365(19)	C(8)-C(9)	1.477(3)
Cd(1)-O(4)#1	2.3366(19)	C(9)-C(10)	1.371(4)
Cd(1)-N(1)	2.320(2)	C(9)-C(13)	1.405(3)
Cd(1)-N(1)#1	2.320(2)	C(10)-C(11)	1.407(4)
O(1)-C(8)	1.210(3)	C(11)-C(12)#2	1.369(4)
O(7)-C(26)	1.184(6)	C(12)-C(11)#2	1.369(4)
O(7)-C(26)#1	1.184(6)	C(12)-C(13)	1.409(3)
O(2)-C(7)	1.206(3)	C(13)-C(13)#2	1.417(5)
O(3)-C(14)	1.257(3)	C(14)-C(15)	1.509(3)
O(4)-C(14)	1.248(3)	C(15)-C(16)	1.369(4)
O(5)-C(25)	1.216(4)	C(15)-C(20)	1.426(4)
O(6)-C(25)	1.292(4)	C(16)-C(17)	1.394(4)
N(1)-C(1)	1.338(3)	C(17)-C(18)	1.379(4)
N(1)-C(5)	1.334(3)	C(18)-C(19)	1.422(4)
N(2)-C(6)	1.482(3)	C(18)-C(25)	1.504(4)
N(2)-C(7)	1.396(4)	C(19)-C(20)	1.437(3)
N(2)-C(8)	1.387(3)	C(19)-C(24)	1.423(4)
N(3)-N(3)#1	1.263(12)	C(20)-C(21)	1.416(4)
N(3)-C(26)	1.433(8)	C(21)-C(22)	1.362(5)
N(3)-C(28)	1.382(8)	C(22)-C(23)	1.400(5)
C(1)-C(2)	1.368(4)	C(23)-C(24)	1.360(5)
C(2)-C(3)	1.383(4)	C(26)-C(26)#1	1.706(13)
Symmetry code: #1 1/2-x, +y, -z; #1 -1/2-x, 1/2-y, -1/2-z			
O(7)-Cd(1)-O(3)#1	85.72(4)	O(2)-C(7)-C(12)	123.1(3)
O(7)-Cd(1)-O(3)	85.72(4)	N(2)-C(7)-C(12)	116.6(2)
O(7)-Cd(1)-O(4)	137.58(4)	O(1)-C(8)-N(2)	120.4(2)

O(7)-Cd(1)-O(4)#1	137.58(4)	O(1)-C(8)-C(9)	122.3(3)
O(3)-Cd(1)-O(3)#1	171.43(8)	N(2)-C(8)-C(9)	117.3(2)
O(4)#1-Cd(1)-O(3)	135.62(6)	C(10)-C(9)-C(8)	120.5(2)
O(4)#1-Cd(1)-O(3)#1	52.81(6)	C(10)-C(9)-C(13)	120.1(2)
O(4)-Cd(1)-O(3)#1	135.62(6)	C(13)-C(9)-C(8)	119.5(2)
O(4)-Cd(1)-O(3)	52.81(6)	C(9)-C(10)-C(11)	120.8(3)
O(4)-Cd(1)-O(4)#1	84.84(9)	C(12)#2-C(11)-C(10)	120.1(2)
N(1)#1-Cd(1)-O(7)	80.92(6)	C(11)#2-C(12)-C(7)	119.9(2)
N(1)-Cd(1)-O(7)	80.92(6)	C(11)#2-C(12)-C(13)	120.3(2)
N(1)#1-Cd(1)-O(3)	85.23(7)	C(13)-C(12)-C(7)	119.8(2)
N(1)-Cd(1)-O(3)	93.41(7)	C(9)-C(13)-C(12)	121.3(2)
N(1)#1-Cd(1)-O(3)#1	93.42(7)	C(9)-C(13)-C(13)#2	119.4(3)
N(1)-Cd(1)-O(3)#1	85.23(7)	C(12)-C(13)-C(13)#2	119.3(3)
N(1)-Cd(1)-O(4)#1	101.51(7)	O(3)-C(14)-C(15)	121.5(2)
N(1)#1-Cd(1)-O(4)	101.51(7)	O(4)-C(14)-O(3)	121.6(2)
N(1)-Cd(1)-O(4)	91.91(7)	O(4)-C(14)-C(15)	116.9(2)
N(1)#1-Cd(1)-O(4)#1	91.92(7)	C(16)-C(15)-C(14)	116.1(2)
N(1)-Cd(1)-N(1)#1	161.84(11)	C(16)-C(15)-C(20)	119.6(2)
C(26)#1-O(7)-Cd(1)	133.9(3)	C(20)-C(15)-C(14)	124.3(2)
C(26)-O(7)-Cd(1)	133.9(3)	C(15)-C(16)-C(17)	121.5(2)
C(26)#1-O(7)-C(26)	92.2(7)	C(18)-C(17)-C(16)	121.0(3)
C(14)-O(3)-Cd(1)	87.31(14)	C(17)-C(18)-C(19)	119.7(2)
C(14)-O(4)-Cd(1)	97.95(15)	C(17)-C(18)-C(25)	117.0(3)
C(1)-N(1)-Cd(1)	119.88(17)	C(19)-C(18)-C(25)	123.3(3)
C(5)-N(1)-Cd(1)	121.22(17)	C(18)-C(19)-C(20)	119.1(2)
C(5)-N(1)-C(1)	118.2(2)	C(18)-C(19)-C(24)	123.2(2)
C(7)-N(2)-C(6)	116.8(2)	C(24)-C(19)-C(20)	117.7(3)
C(8)-N(2)-C(6)	118.0(2)	C(15)-C(20)-C(19)	119.1(2)
C(8)-N(2)-C(7)	125.2(2)	C(21)-C(20)-C(15)	122.1(2)
N(3)#1-N(3)-C(26)	98.9(4)	C(21)-C(20)-C(19)	118.7(2)
N(3)#1-N(3)-C(28)	145.8(6)	C(22)-C(21)-C(20)	121.3(3)
C(28)-N(3)-C(26)	115.4(7)	C(21)-C(22)-C(23)	120.1(3)

N(1)-C(1)-C(2)	122.3(3)	C(24)-C(23)-C(22)	120.8(3)
C(1)-C(2)-C(3)	119.0(3)	C(23)-C(24)-C(19)	121.3(3)
C(4)-C(3)-C(2)	119.7(3)	O(5)-C(25)-O(6)	121.8(3)
C(3)-C(4)-C(5)	117.2(2)	O(5)-C(25)-C(18)	125.2(3)
C(3)-C(4)-C(6)	121.8(2)	O(6)-C(25)-C(18)	112.4(3)
C(5)-C(4)-C(6)	121.0(2)	O(7)-C(26)-N(3)	125.0(6)
N(1)-C(5)-C(4)	123.5(2)	O(7)-C(26)-C(26)#1	43.9(3)
N(2)-C(6)-C(4)	113.3(2)	N(3)-C(26)-C(26)#1	81.1(4)
O(2)-C(7)-N(2)	120.3(3)		
Symmetry code: #1 1/2-x, +y, -z; #2 -1/2-x, 1/2-y, -1/2-z			
Compound **2**			
Cd(1)-O(1)	2.247(5)	N(1)-C(1)	1.318(10)
Cd(1)-O(2)#1	2.282(6)	N(1)-C(5)	1.326(9)
Cd(1)-O(3)#2	2.400(6)	N(2)-C(6)	1.480(10)
Cd(1)-O(4)#2	2.409(6)	N(2)-C(7)	1.387(10)
Cd(1)-N(1)	2.344(6)	N(3)-C(19)	1.395(13)
Cd(1)-N(4)#3	2.318(6)	N(3)-C(20)	1.384(14)
Cd(1)-C(38)#2	2.732(9)	N(4)-C(24)	1.342(11)
O(1)-C(27)	1.261(9)	N(4)-C(25)	1.322(10)
O(2)-Cd(1)#1	2.282(6)	C(1)-C(2)	1.388(11)
O(3)-C(38)	1.225(10)	C(2)-C(3)	1.362(10)
O(4)-Cd(1)#4	2.409(6)	C(3)-C(4)	1.376(10)
O(4)-C(38)	1.256(10)	C(3)-C(6)	1.498(11)
O(5)-C(8)	1.220(9)	O(9)-C(39)	1.28(2)
O(6)-C(7)	1.207(9)	O(9)-C(39A)	1.23(2)
O(7)-C(19)	1.208(11)		
Symmetry code: #1 -x, 1-y, 1-z; #2 -1/2+x, 1-y, 1/2-z; #3 +x, 1+y, +z; #4 1/2+x, 1-y, 1/2-z			
O(1)-Cd(1)-O(2)#1	118.9(2)	C(10)-C(15)-C(14)	118.7(9)
O(1)-Cd(1)-O(3)#2	94.4(2)	C(10)-C(15)-C(16)	119.2(8)
O(1)-Cd(1)-O(4)#2	148.2(2)	C(16)-C(15)-C(14)	122.1(8)
O(1)-Cd(1)-N(1)	87.2(2)	C(15)-C(16)-C(20)	118.7(10)
O(1)-Cd(1)-N(4)#3	95.3(2)	C(17)-C(16)-C(15)	120.4(8)

O(1)-Cd(1)-C(38)#2	120.9(3)	C(16)-C(17)-C(18)	121.3(8)
N(1)-Cd(1)-O(3)#2	81.6(2)	C(9)-C(18)-C(17)	119.6(8)
N(1)-Cd(1)-O(4)#2	89.1(2)	C(33)-C(28)-C(27)	123.6(7)
N(1)-Cd(1)-C(38)#2	82.7(2)	C(28)-C(29)-C(30)	121.9(7)
N(4)#3-Cd(1)-O(3)#2	101.5(2)	C(31)-C(30)-C(29)	120.5(8)
N(4)#3-Cd(1)-O(4)#2	90.5(2)	C(30)-C(31)-C(32)	120.0(7)
N(4)#3-Cd(1)-N(1)	175.7(2)	C(30)-C(31)-C(38)	118.4(7)
N(4)#3-Cd(1)-C(38)#2	98.8(2)	C(32)-C(31)-C(38)	121.6(7)
C(27)-O(1)-Cd(1)	124.4(5)	C(31)-C(32)-C(33)	118.9(7)
C(27)-O(2)-Cd(1)#1	148.1(5)	C(37)-C(32)-C(31)	122.1(7)
C(5)-N(1)-Cd(1)	117.7(5)	C(37)-C(32)-C(33)	118.9(7)
C(7)-N(2)-C(6)	116.7(7)	C(32)-C(33)-C(28)	120.5(7)
C(1)-N(1)-Cd(1)	124.0(5)	C(34)-C(33)-C(28)	121.7(7)
C(1)-N(1)-C(5)	116.6(7)	C(34)-C(33)-C(32)	117.7(7)
C(17)-C(16)-C(20)	121.0(10)	C(35)-C(34)-C(33)	121.0(8)

Symmetry code: #1 -x, 1-y, 1-z; #2 -1/2+x, 1-y, 1/2-z; #3 +x, 1+y, +z; #3 1/2+x, 1-y, 1/2-z;

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

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(3)-H(3)...O(1)	0.93	2.44	3.361(4)	173
C(5)-H(5)...O(2)	0.93	2.55	3.238(3)	131
C(6)-H(6A)...O(2)	0.97	2.34	2.688(4)	100
C(17)-H(17)...O(6)	0.93	2.29	2.642(4)	102