Electronic Supplementary Material (ESI) for Dalton Transactions.

This journal is © The Royal Society of Chemistry 2021

A Naphthalene Diimide-based Metal-organic Framework as An Electron-deficient Platform with Photochromic and Chemochromic Properties

Bohong Gao, Pengfei Hao,* Gao-Peng 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, Linfen 041004, China.

Supplementary Information Contents

1. Figures

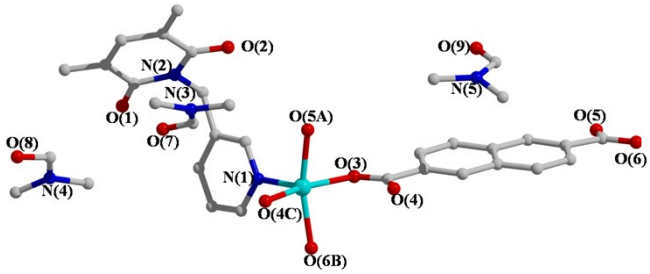

Fig. S1 The asymmetric unit of **1@DMF** (symmetry codes: A: x, 0.5-y, -0.5+z; B: 2-x, 0.5+y, 1.5-z; C: 2-x, 1-y, 1-z.).

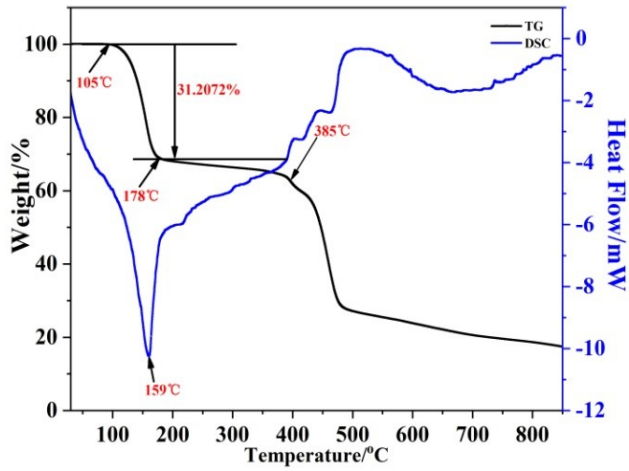

Fig. 2 Thermo-gravimetric (TG) and Differential scanning calorimetry (DSC) curves of **1@DMF**.

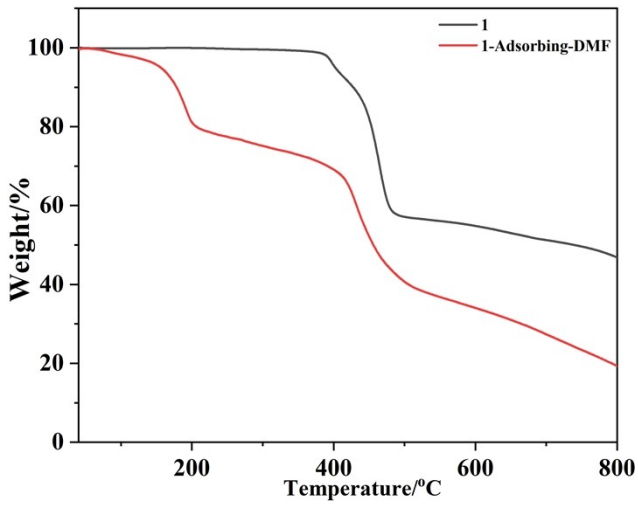

Fig. S3 TG curve of **1** and **1-Adsorbing DMF**.

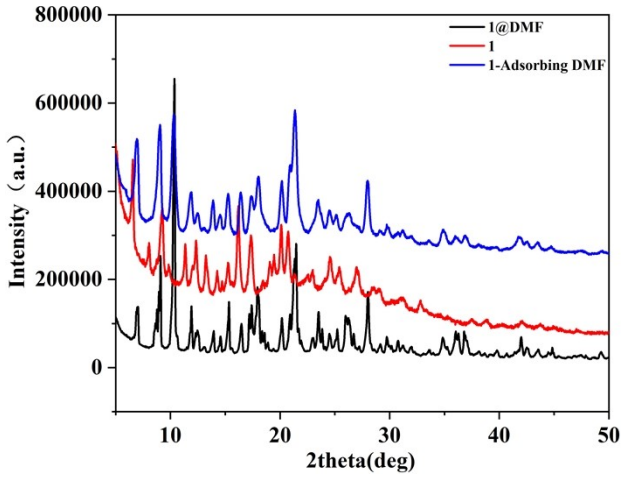

Fig. S4 Powder X-ray diffraction (PXRD) patterns for **1@DMF**, **1** and **1-Adsorbing DMF** at room temperature.

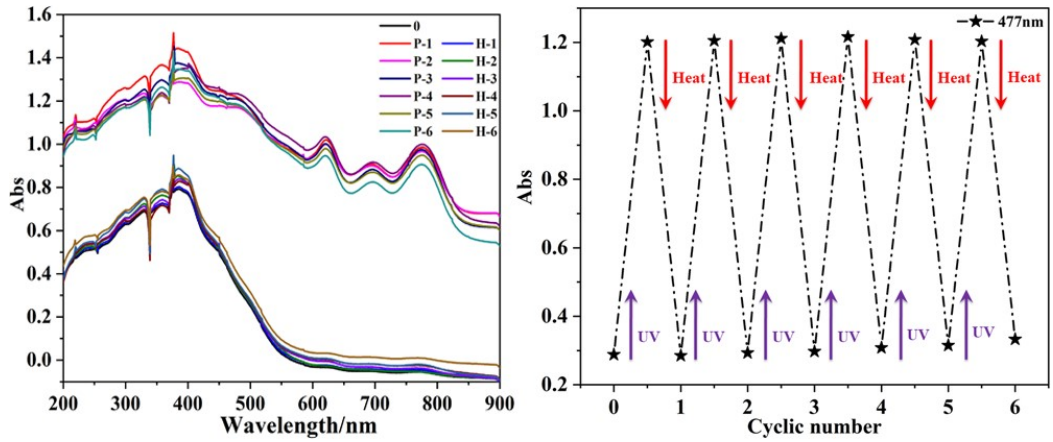

Fig. S5 The UV-vis absorption spectra and switching cycles of coloration-decoloration processes of **1@DMF** (477nm) upon alternating UV light illumination and thermal treatment.

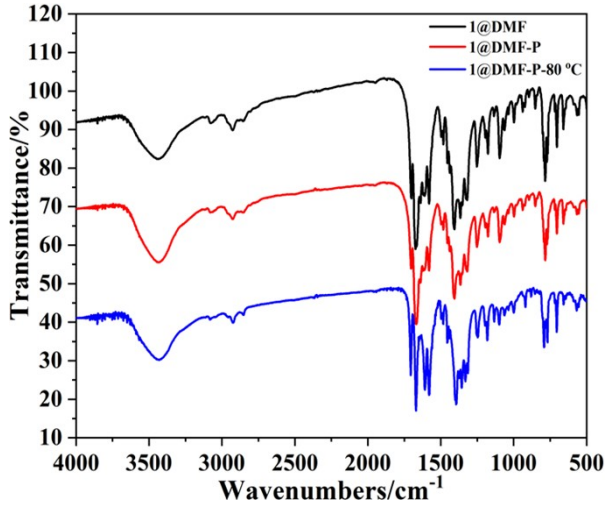

Fig. S6 IR spectra of **1@DMF**, **1@DMF-P** and **1@DMF-P-80 °C**.

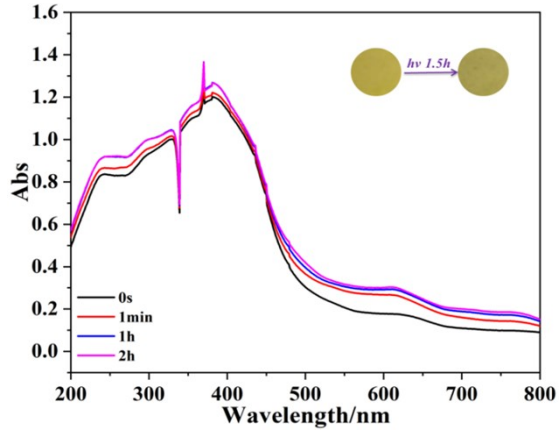

Fig. S7 UV-vis absorption spectra of **1**.

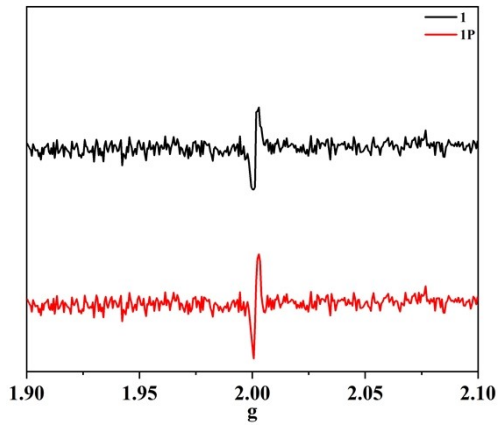

Fig. S8 EPR spectra of **1** and **1P**.

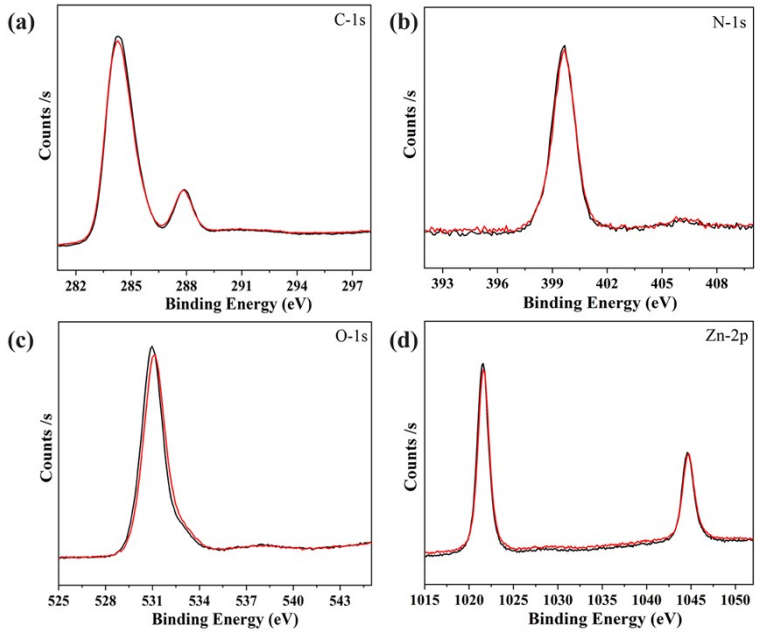

Fig. S9 The XPS core-level spectra of **1** and **1P** before and after UV light irradiation at room temperature.

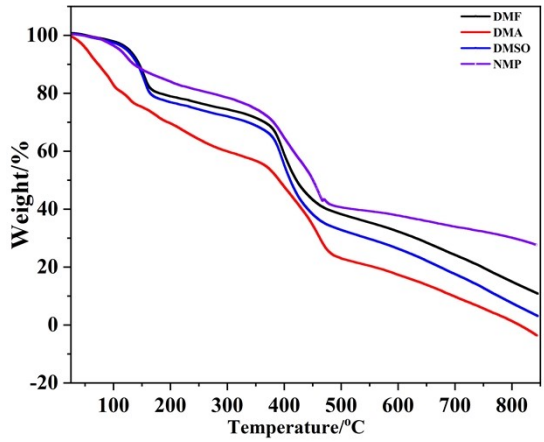

Fig. S10 TG spectra of **1@DMA**, **1@DMSO**, **1@NMP** and **1-Adsorbing DMF**.

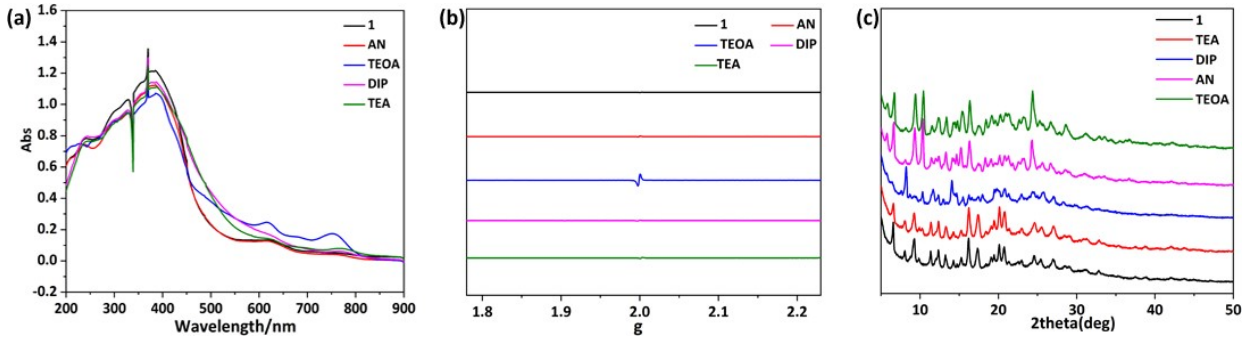

Fig. S11 UV-Vis absorption spectra (a), EPR spectra (b) and PXRD spectra (c) of **1@amines** (amines=AN, TEOA, DIP, TEA).

2. Tables

Table S1. Crystallographic data and refinement of **1@DMF**.

Compounds	**1@DMF**
CCDC code	2052963
Temperature (K)	273(2)
Empirical formula	$C_{34}H_{35}N_5O_9Zn$
Formula weight	723.04
Crystal size (mm)	0.673 × 0.398 × 0.078
Crystal system	monoclinic
Space group	$P2_1/c$
a (Å)	10.4323(13)
b (Å)	19.699(3)
c (Å)	17.150(2)
α (°)	90
β (°)	101.046(3)
γ (°)	90
V (Å^3)	3459.1(7)
Z	4
D_c (g cm^{-3})	1.388
F(000)	1504.0
μ(mm^{-1})	0.771
Reflections collected	50746
Independent reflections	8609
R_{int}	0.0232
Goodness-of-fit on F^2	1.074
R_1/wR_2, [$I \geq 2\sigma(I)$][a,b]	0.0406/ 0.1243
R_1/wR_2, (all data)	0.0536/ 0.1399

Table S2. Selected bond lengths (Å) and angles (°) for **1@DMF**.

1@DMF			
Zn(1)-Zn(1) #1	2.9684(5)	C(12)-C(13)#6	1.398(4)
Zn(1)-O(3)	2.0313(14)	C(13)-C(12)#6	1.399(4)
Zn(1)-O(4)#1	2.0454(15)	C(14)-C(15)	1.505(2)
Zn(1)-O(5)#2	2.0434(14)	C(15)-C(16)	1.410(3)
Zn(1)-O(6)#3	2.0442(14)	C(15)-C(20)	1.370(3)
Zn(1)-N(1)	2.0319(18)	C(16)-C(17)	1.363(3)
O(1)-C(7)	1.206(4)	C(17)-C(18)	1.420(3)
O(2)-C(8)	1.214(3)	C(18)-C(19)	1.415(3)
O(3)-C(14)	1.256(3)	C(18)-C(24)	1.415(3)
O(4)-Zn(1)#1	2.0453(14)	C(19)-C(20)	1.416(3)
O(4)-C(14)	1.250(3)	C(19)-C(21)	1.419(3)
O(5)-Zn(1)#4	2.0435(14)	C(21)-C(22)	1.361(3)
O(5)-C(25)	1.258(3)	C(22)-C(23)	1.412(3)
O(6)-Zn(1)#5	2.0441(14)	C(23)-C(24)	1.370(3)
O(6)-C(25)	1.251(3)	C(23)-C(25)	1.501(2)
N(1)-C(1)	1.332(3)	O(7)-C(28)	1.202(7)
N(1)-C(5)	1.339(3)	N(3)-C(26)	1.442(7)
N(2)-C(6)	1.476(3)	N(3)-C(27)	1.375(5)
N(2)-C(7)	1.394(4)	N(3)-C(28)	1.341(6)
N(2)-C(8)	1.387(3)	O(8)-C(31)	1.248(9)
C(1)-C(2)	1.373(4)	N(4)-C(29)	1.430(7)
C(2)-C(3)	1.379(5)	N(4)-C(30)	1.351(8)
C(3)-C(4)	1.366(4)	N(4)-C(31)	1.367(6)
C(4)-C(5)	1.383(3)	O(9)-C(33)	1.192(7)
C(4)-C(6)	1.506(4)	N(5)-C(32)	1.468(8)
C(7)-C(11)	1.484(4)	N(5)-C(33)	1.426(7)
C(8)-C(9)	1.480(4)	N(5)-C(34)	1.427(8)
C(9)-C(10)	1.406(4)	O(9A)-C(33A)	1.215(8)
C(9)-C(13)	1.374(4)	N(5A)-C(32A)	1.476(8)
C(10)-C(10)#6	1.416(5)	N(5A)-C(33A)	1.421(8)
C(10)-C(11)	1.405(4)	N(5A)-C(34A)	1.447(8)
C(11)-C(12)	1.370(4)		
O(3)-Zn(1)-Zn(1)#1	84.82(5)	C(10)-C(11)-C(7)	119.4(3)
O(3)-Zn(1)-O(4)#1	159.04(7)	C(12)-C(11)-C(7)	120.2(3)
O(3)-Zn(1)-O(5)#2	87.54(7)	C(12)-C(11)-C(10)	120.4(3)
O(3)-Zn(1)-O(6)#3	89.48(8)	C(11)-C(12)-C(13)#6	120.5(3)
O(3)-Zn(1)-N(1)	103.63(7)	C(9)-C(13)-C(12)#6	120.4(3)

O(4)#1-Zn(1)-Zn(1)#1	74.22(5)	O(3)-C(14)-C(15)	117.13(19)
O(5)#2-Zn(1)-Zn(1)#1	79.39(5)	O(4)-C(14)-O(3)	125.70(18)
O(5)#2-Zn(1)-O(4)#1	88.47(8)	O(4)-C(14)-C(15)	117.17(18)
O(5)#2-Zn(1)-O(6)#3	159.25(7)	C(16)-C(15)-C(14)	120.28(19)
O(6)#3-Zn(1)-Zn(1)#1	79.90(5)	C(20)-C(15)-C(14)	119.79(19)
O(6)#3-Zn(1)-O(4)#1	87.01(7)	C(20)-C(15)-C(16)	119.92(18)
N(1)-Zn(1)-Zn(1)#1	171.52(6)	C(17)-C(16)-C(15)	120.8(2)
N(1)-Zn(1)-O(4)#1	97.33(7)	C(16)-C(17)-C(18)	120.5(2)
N(1)-Zn(1)-O(5)#2	101.46(7)	C(19)-C(18)-C(17)	118.93(18)
N(1)-Zn(1)-O(6)#3	99.20(7)	C(19)-C(18)-C(24)	118.90(19)
C(14)-O(3)-Zn(1)	120.84(14)	C(24)-C(18)-C(17)	122.17(19)
C(14)-O(4)-Zn(1)#1	134.39(14)	C(18)-C(19)-C(20)	119.06(19)
C(25)-O(5)-Zn(1)#4	127.55(13)	C(18)-C(19)-C(21)	118.79(19)
C(25)-O(6)-Zn(1)#5	126.88(14)	C(20)-C(19)-C(21)	122.2(2)
C(10)-C(9)-C(8)	119.8(2)	C(34)-N(5)-C(32)	118.4(7)
C(13)-C(9)-C(8)	120.1(3)	O(9)-C(33)-N(5)	122.1(10)
C(13)-C(9)-C(10)	120.1(3)	C(33A)-N(5A)-C(32A)	108.1(9)
C(9)-C(10)-C(10)#6	119.4(3)	C(33A)-N(5A)-C(34A)	138.5(12)

[1]2-X,1-Y,1-Z; [2]+X,1/2-Y,-1/2+Z; [3]2-X,1/2+Y,3/2-Z; [4]+X,1/2-Y,1/2+Z; [5]2-X,-1/2+Y,3/2-Z; [6]1-X,1-Y,-Z

Table S3. Hydrogen bonds of for **1@DMF** (Å and °).

Compound **1@DMF**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(1)-H(1) ... O(6)	0.930	2.580	3.164	121.22
C(5)-H(5) ... O(2)	0.930	2.605	3.276	129.47
C(26)-H(26A) ... O(1)	0.960	2.605	3.258	125.49
C(29)-H(29A) ... O(7)	0.960	2.474	3.432	175.51
C(32)-H(32C) ... O(8)	0.960	2.620	3.396	138.06
#1 -x+2, y+1/2, -z+3/2;#2 x+1, y, z;#3 -x+2, y-1/2, -z+1/2				