Electronic Supplementary Information

Different photochromic properties induced by lone pair-π interactions varying strength in two stereocontrolled self-assembly isomeric coordination polymers†

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1. Graphics

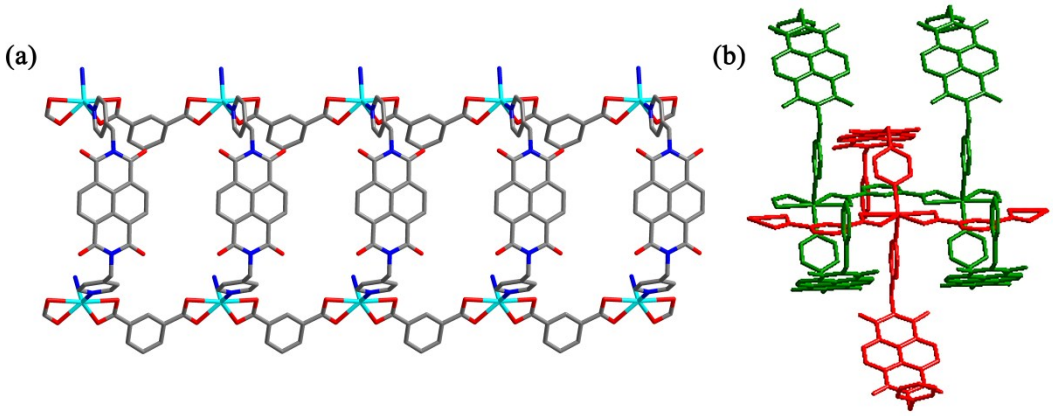

Fig. S1 (a) Selected part of 2D structure showing the connection mode of m-BDC^{2-} ligand and (b) interpenetrated two kinds directional unit construction structures in compound **1**.

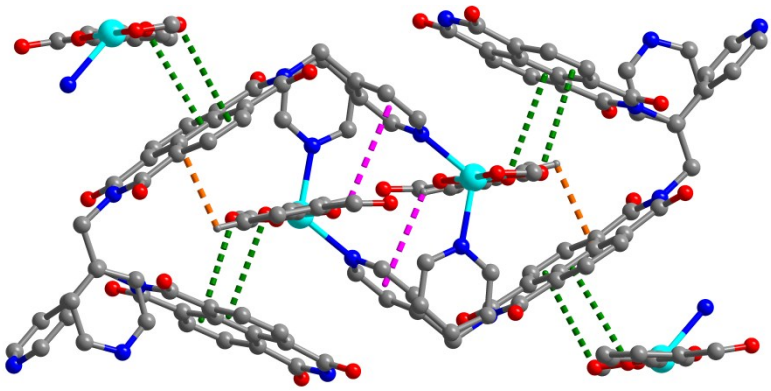

Fig. S2 The interactions (green: lone pair-π interactions; orange and pink: CH-π interactions) between different molecules from 2D networks forming 3D supramolecular structure in compound **1**.

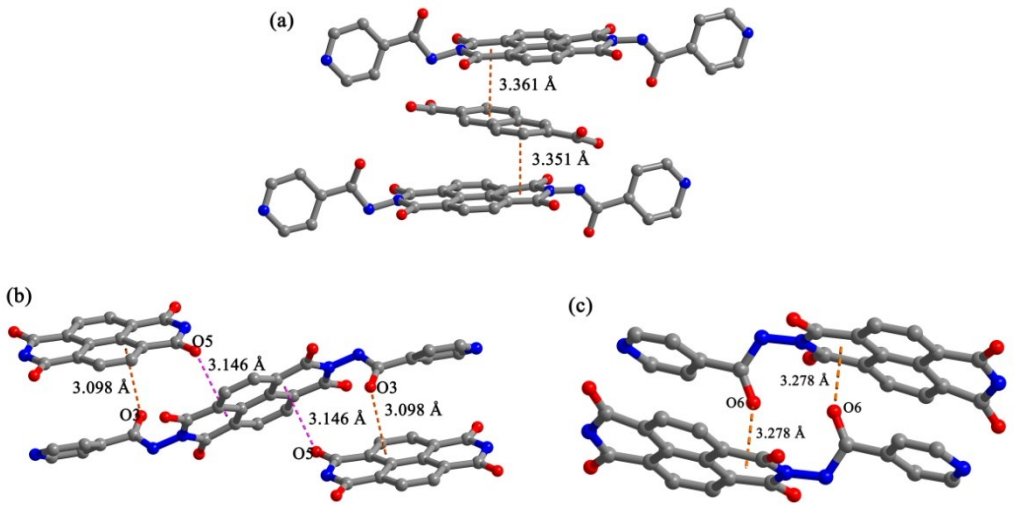

Fig. S3 (a) Face-to-face π-π stacking interactions in the adopted framework [Cd(IsoNDI)(2,6-NDC)(H_2O)$_2$]; Lone pair-π interactions between adjacent IsoNDI ligands in the two adopted frameworks [Cd(IsoNDI)(m-BDC)(DMF)] (b) and [Cd_2(IsoNDI)$_2$(p-BDC)$_{0.5}$($MAC)_2$] (c) .

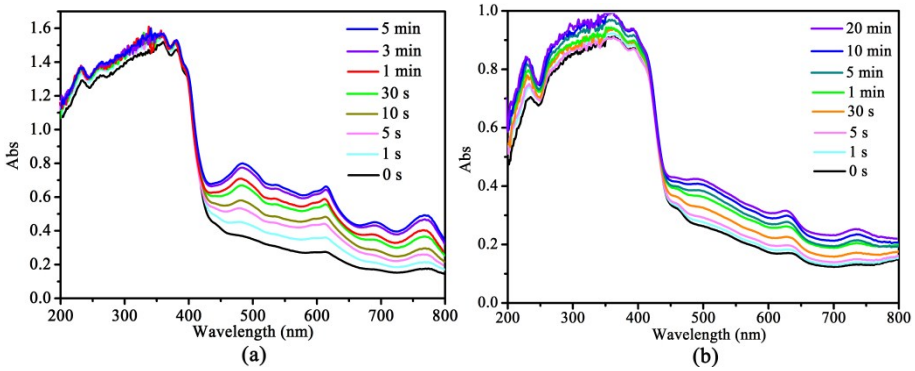

Fig. S4 Time-dependent UV-Vis spectra of compounds **1** (a) and **2** (b) upon irradiation by 300W xenon lamp.

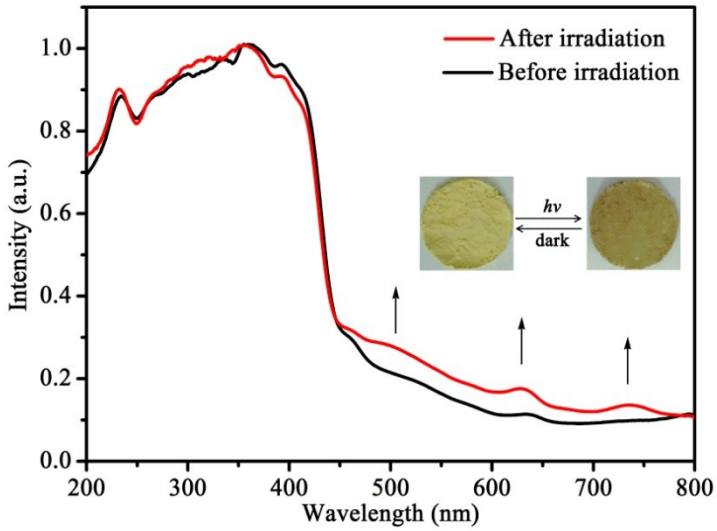

Fig. S5 UV-Vis spectrum of DPMNI free ligand before and after irradiation by 300W xenon lamp.

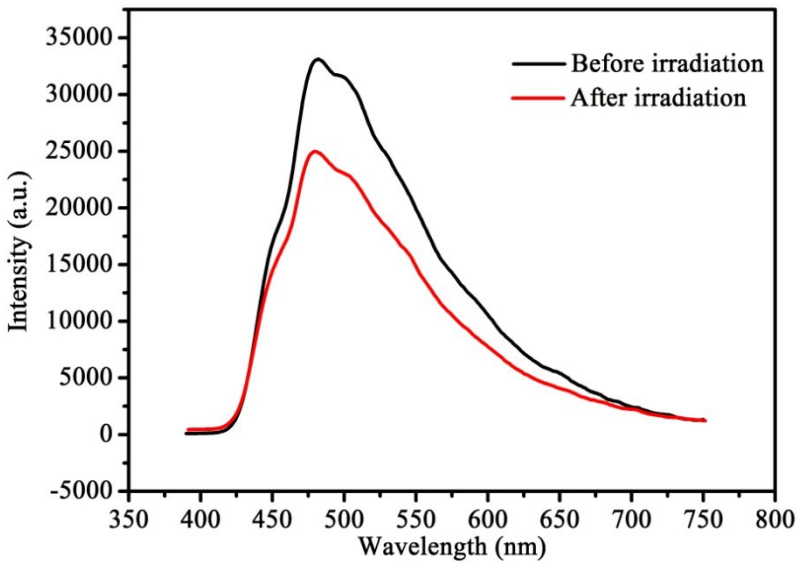

Fig. S6 Luminescence spectrum of DPMNI free ligand before and after irradiation by 300W xenon lamp.

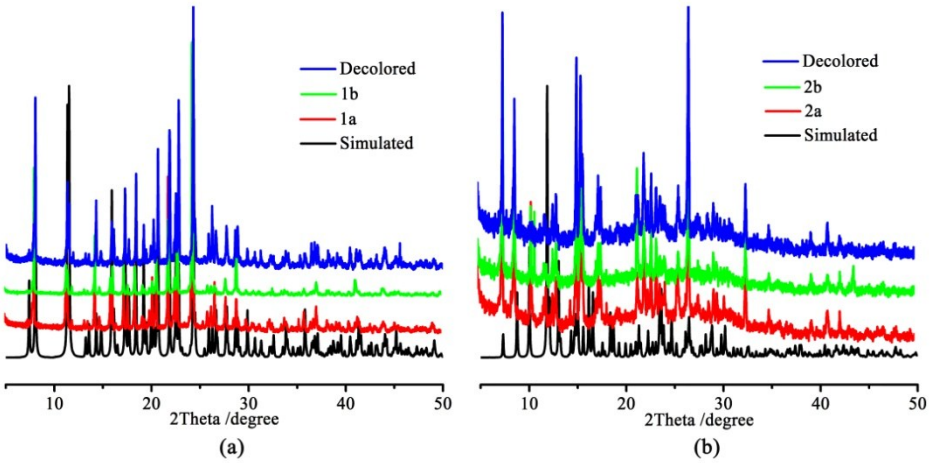

Fig. S7 PXRD patterns of compounds **1** (a) and **2** (b). Lables: **1a**, **2a**: before irradiation; **1b**, **2b**: after irradiation; **Decolored**: by dark treatment about one month; **Simulated**: according to their single-crystal X-ray diffraction data.

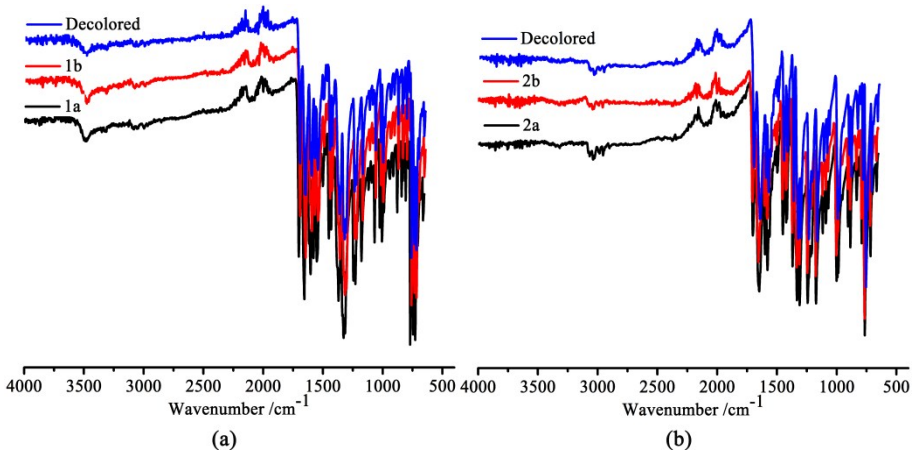

Fig. S8 IR spectra of compounds **1** (a) and **2** (b). Lables: **1a**, **2a**: before irradiation; **1b**, **2b**: after irradiation; **Decolored**: by dark treatment about one month;

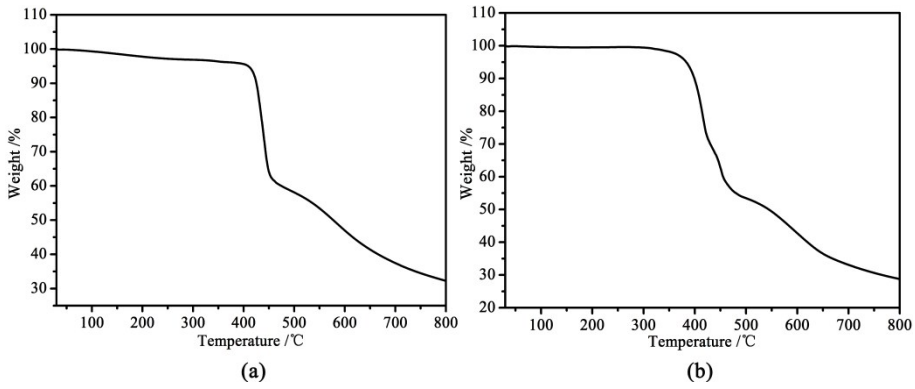

Fig. S9 TGA curves of compounds **1** (a) and **2** (b) were carried out in powder states under N_2 atmosphere.

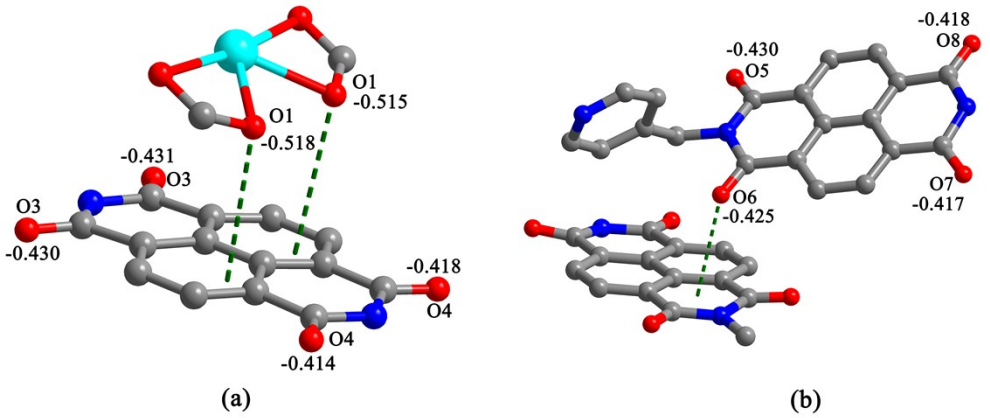

Fig. S10 The charge of different O atoms in two kinds lone pair-π interactions as electron transfer pathways in compounds **1** (a)-**2** (b).

2. Tables

Table S1. Crystal data and structure refinement parameters for compounds **1-2**

Compound	**1**	**2**
Empirical formula	$C_{34}H_{20}N_4O_8Cd$	$C_{34}H_{20}N_4O_8Cd$
Formula weight	724.94	724.94
Crystal system	Orthorhombic	Monoclinic
Space group	Pnma	P21/n
a (Å)	23.835(5)	18.0496(10)
b(Å)	10.0215(19)	8.0270(4)
c (Å)	12.362(2)	20.6646(11)
α (°)	90	90
β (°)	90	102.2210(10)
γ (°)	90	90
V (Å^3)	2952.7(10)	2926.1(3)
Z	4	4
T (K)	296(2)	296(2)
ρ_{calc} (g/cm^3)	1.631	1.646
F (000)	1456	1456
Absorption coefficient	0.802	0.810
Goodness-of-fit on F^2	0.753	1.017
$R_1{}^a$, $wR_2{}^b$ ($I > 2\sigma(I)$)	0.0478, 0.1614	0.0297, 0.0433
$R_1{}^a$, $wR_2{}^b$ (*all data*)	0.0583, 0.1777	0.0654, 0.0724

$^aR_1 = \sum \| F_0 | - | F_c \| / \sum | F_0 |$. $^bwR_2 = [\sum w(F_0^2 - F_c^2)^2 / \sum w(F_0^2)]^{1/2}$.

Table S2. Selected Bond lengths [Å] and angles [°] for compounds **1-2**

Compound 1	**Compound 2**
Cd(1)-N(4)#2 2.256(5)	Cd(1)-N(4)#1 2.313(2)
Cd(1)-N(1) 2.254(5)	Cd(1)-N(1) 2.295(2)
Cd(1)-O(1) 2.266(4)	Cd(1)-O(1) 2.399(2)
Cd(1)-O(2) 2.512(5)	Cd(1)-O(2) 2.298(2)
Cd(1)-O(1)#1 2.266(4)	Cd(1)-O(3) 2.315(2)
Cd(1)-O(2)#1 2.512(5)	Cd(1)-O(4) 2.430(2)
N(4)#2-Cd(1)-O(1)#1 125.80(14)	N(1)-Cd(1)-O(2) 97.68(9)
N(4)#2-Cd(1)-O(1) 125.80(14)	O(2)-Cd(1)-O(3) 104.12(9)
O(1)-Cd(1)-O(1)#1 79.7(2)	O(3)-Cd(1)-N(1) 105.81(8)
N(4)#2-Cd(1)-N(1) 116.12(17)	N(4)#1-Cd(1)-O(2) 109.69(9)
N(1)-Cd(1)-O(1)#1 100.86(17)	N(1)-Cd(1)-N(4)#1 98.97(9)
N(1)-Cd(1)-O(1) 100.86(17)	N(4)#1-Cd(1)-O(3) 134.5(2)
N(4)#2-Cd(1)-O(2)#1 86.83(9)	O(2)-Cd(1)-O(1) 55.73(9)
O(1)#1-Cd(1)-O(2)#1 53.90(13)	N(1)-Cd(1)-O(1) 151.54(9)
O(1)-Cd(1)-O(2)#1 133.64(14)	O(1)-Cd(1)-O(3) 91.89(8)
N(1)-Cd(1)-O(2)#1 89.52(10)	N(4)#1-Cd(1)-O(1) 83.10(8)
N(4)#2-Cd(1)-O(2) 86.83(9)	O(4)-Cd(1)-O(2) 158.83(9)
O(2)-Cd(1)-O(1)#1 133.64(14)	N(1)-Cd(1)-O(4) 86.54(8)
O(1)-Cd(1)-O(2) 53.90(13)	O(3)-Cd(1)-O(4) 54.96(8)
N(1)-Cd(1)-O(2) 89.52(10)	N(4)#1-Cd(1)-O(4) 89.96(8)
O(2)#1-Cd(1)-O(2) 172.41(17)	O(1)-Cd(1)-O(4) 121.91(9)

Symmetry code: for **1**: #1: x, 0.5-y, z; #2: -0.5+x, y, 0.5-z. for **2**: #1: -0.5+x, 1.5-y, 0.5+z.