Electronic Supplementary Material (ESI) for CrystEngComm

Effect of iodide on the electronic and photoresponsive behaviors of 1D naphthalenediimide-based zinc coordination polymers

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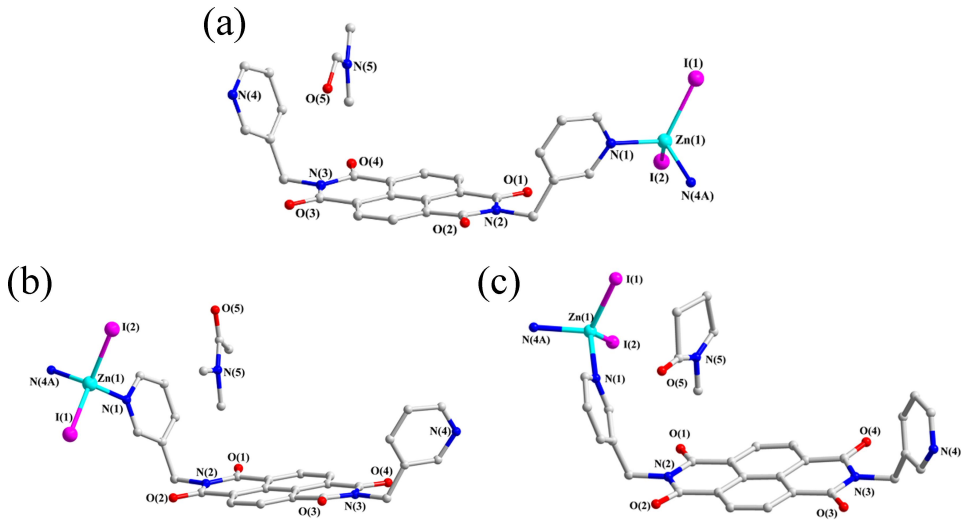

Fig. S1 (a) Coordination environment of Zn^{2+} in **2** (symmetry codes: A：*0.5+x*, *0.5-y*, *-0.5+z*;). (b) Coordination environment of Zn^{2+} in **3** (symmetry codes: A：*-0.5+x*, *1.5-y*, *0.5+z*;). (c) Coordination environment of Zn^{2+} in **4** (symmetry codes: A：*-0.5+x*, *1.5-y*, *0.5+z*;). All hydrogen atoms are omitted for clarity.

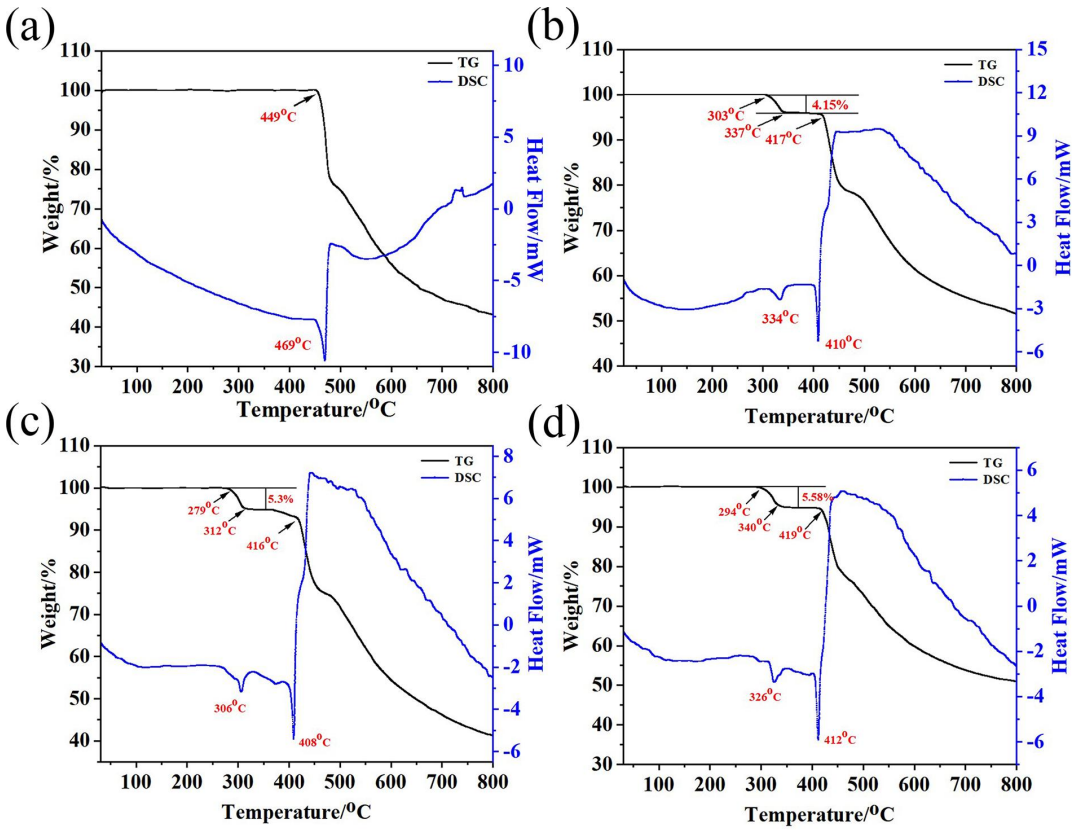

Fig. S2 Thermo-gravimetric (TG) and Differential scanning calorimetry (DSC) curves of **1**-**4**.

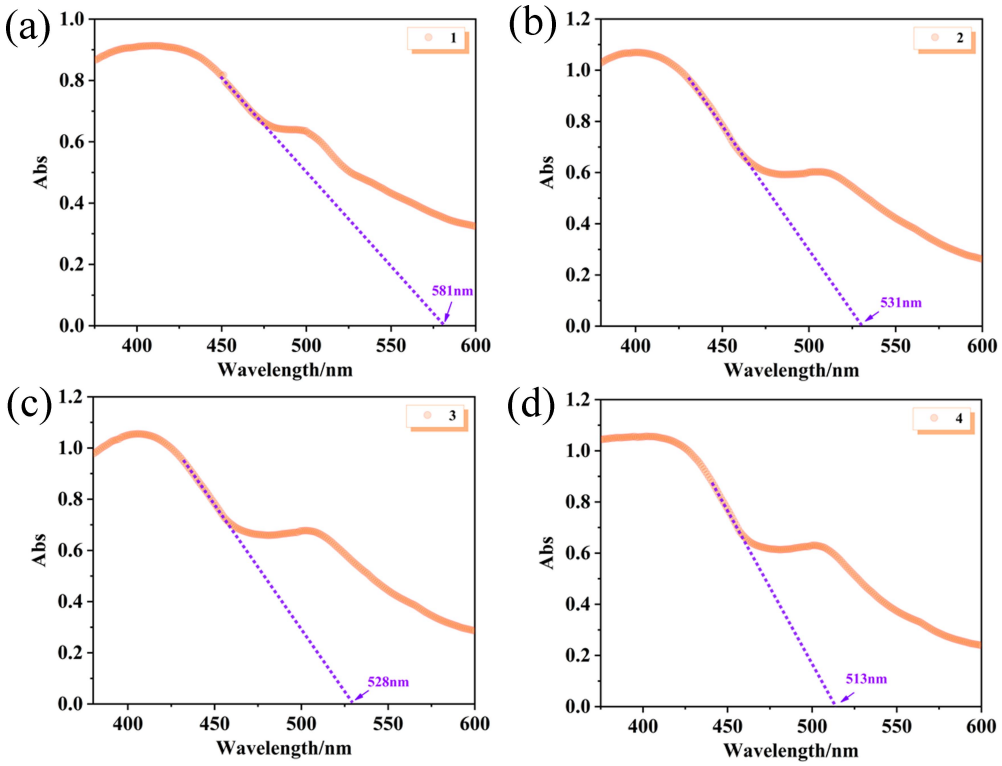

Fig. S3 Kubelka-Munk transformed reflectivity vs energy of complexes **1**-**4**.

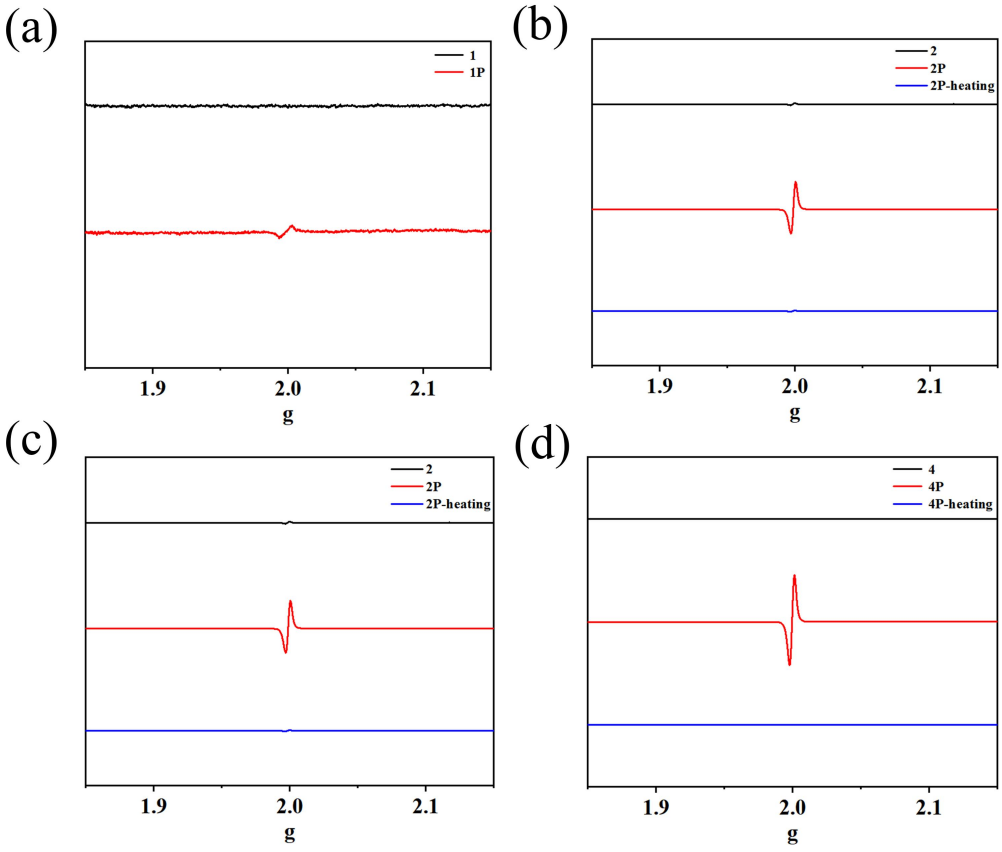

Fig. S4 The EPR spectra of **1** and **1P** (a), **2**, **2P** and **2P**-heating (b), **3**, **3P**and **3P**-heating (c) and **4**, **4P**and **4P**-heating (d).

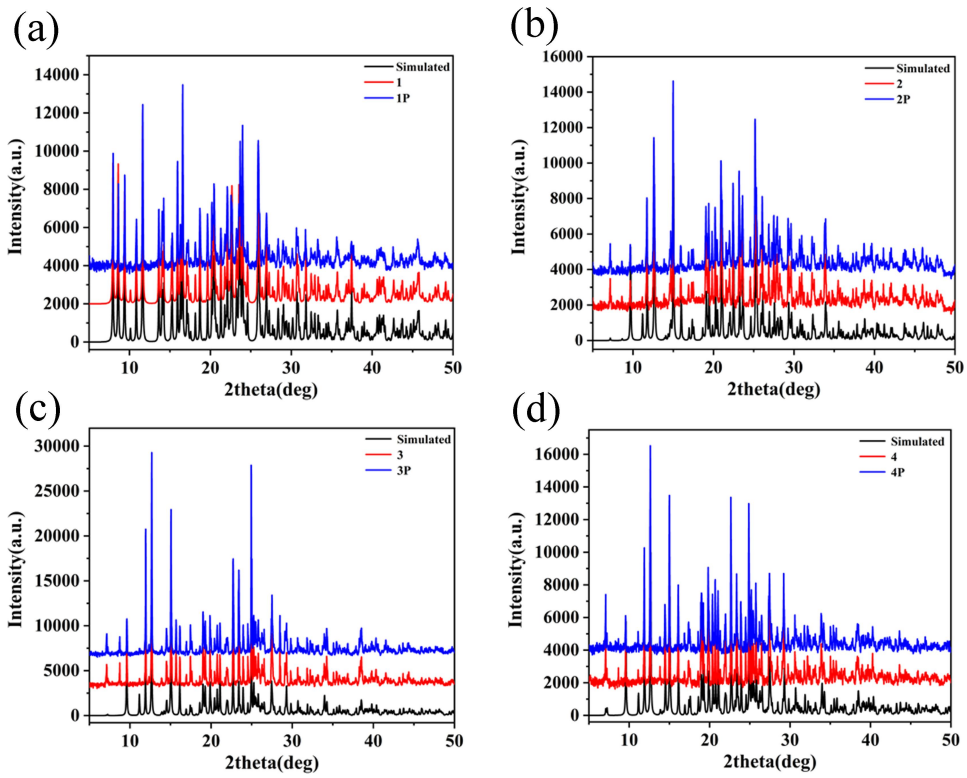

Fig. S5 PXRD patterns of **1**-**4** simulated from the X-ray single-crystal structures, as-synthesized samples and after irradiation samples.

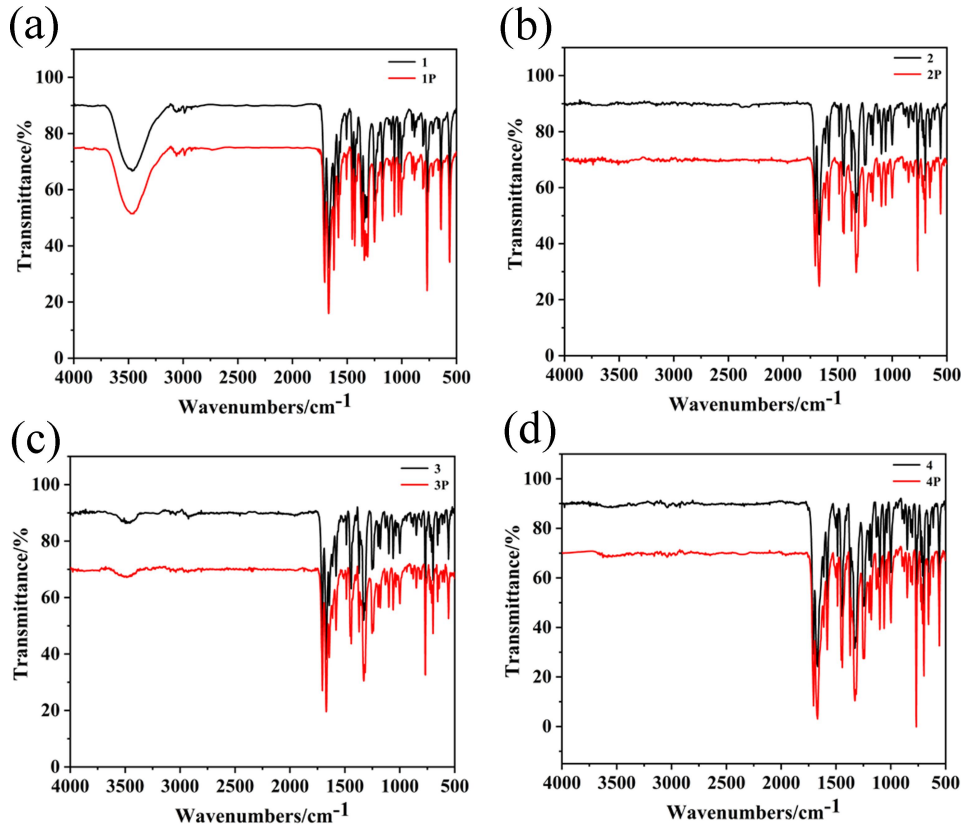

Fig. S6 FT-IR spectra of **1**-**4** as-synthesized samples and after irradiation samples.

2. Tables

Table S1 Crystallographic data and refinement of **1**-**4.**

Compound	**1**	**2**	**3**	**4**
CCDC code	2349645	2349646	2349647	2349648
Temperature (K)	293(2)	293(2)	293(2)	293(2)
Empirical formula	$C_{26}H_{16}I_2N_4O_4Zn$	$C_{55}H_{39}I_4N_9O_9Zn_2$	$C_{56}H_{41}I_4N_9O_9Zn_2$	$C_{57}H_{41}I_4N_9O_9Zn_2$
Formula weight	767.60	1608.29	1622.32	1634.33
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	*P*-1	*C2/c*	*C2/c*	*C2/c*
a (Å)	10.1573(9)	25.3483(17)	25.493(4)	25.494(3)
b (Å)	12.2406(11)	13.9149(8)	13.949(3)	13.9506(19)
c (Å)	12.6327(12)	16.2708(10)	16.199(3)	16.205(2)
α (°)	115.380(2)	90	90	90
β (°)	93.680(3)	103.754(3)	102.121(6)	102.081(5)
γ (°)	107.830(2)	90	90	90
V (Å^3)	1315.6(2)	5574.5(6)	5631.9(17)	5636.0(13)
Z	2	4	4	4
D_c (g cm^{-3})	1.938	1.916	1.913	1.926
μ (mm^{-1})	3.320	3.140	3.109	3.108
F (000)	736.0	3104.0	3136.0	3160.0
Reflections collected	21144	50128	41656	50537
Independent reflections	6510	6898	7088	6992
R_{int}	0.0382	0.0570	0.0471	0.0448
Goodness-of-fit on F^2	1.005	0.961	1.018	0.932
R_1/wR_2, [$I \geq 2\sigma(I)$][a,b]	0.0465/0.0805	0.0445/0.1268	0.0426/0.0825	0.0373/0.1142
R_1/wR_2, (all data)	0.1023/0.0957	0.0870/0.1501	0.0791/0.0939	0.0629/0.1334

[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 (°) for **1**-**4**.

Compound **1**			
Zn1-I2	2.5508(8)	Zn1-N1	2.0699(4)
Zn1-I1	2.5217(6)	Zn1-N3	2.0518(3)
I1-Zn1-I2	119.94(2)	N3-Zn1-N1	98.10(15)
N1-Zn1-I2	106.04(10)	C5-N1-Zn1	120.63(3)
N1-Zn1-I1	108.02(10)	C1-N1-Zn1	121.97(2)
N3-Zn1-I2	105.21(11)	C18-N3-Zn1	125.09(3)
N3-Zn1-I1	116.89(10)	C14-N3-Zn1	117.76(3)

Compound **2**			
Zn1-I1	2.5332(6)	Zn1-N1	2.0683(3)
Zn1-I2	2.5301(6)	Zn1-N4#1	2.0536(3)
N1-Zn1-I1	109.03(11)	I2-Zn1-I1	120.34(3)
N1-Zn1-I2	109.86(11)	C5-N1-Zn1	117.76(3)
N4#1-Zn1-N1	99.23(15)	C1-N1-Zn1	124.30(3)
N4#1-Zn1-I1	106.30(11)	C23-N4-Zn1#2	124.09(3)
N4#1-Zn1-I2	109.97(10)	C24-N4-Zn1#2	117.63(3)
#1 1/2+x,1/2-y,-1/2+z; #2 -1/2+x,1/2-y,1/2+z			

Compound **3**			
Zn1-I2	2.5396(7)	Zn1-N1	2.0541(3)
Zn1-I1	2.5308(7)	Zn1-N4#1	2.0667(3)
I1-Zn1-I2	120.29(2)	N4#1-Zn1-I1	109.34(9)
N1-Zn1-I2	107.83(9)	C5-N1-Zn1	124.54(2)
N1-Zn1-I1	109.61(9)	C1-N1-Zn1	117.38(2)
N1-Zn1-N4#1	99.21(13)	C23-N4-Zn1#2	118.04(3)
N4#1-Zn1-I2	108.50(9)	C24-N4-Zn1#2	124.10(3)
#1 -1/2+x,3/2-y,1/2+z; #2 1/2+x,3/2-y,-1/2+z			

Compound **4**			
Zn1-I1	2.5423(6)	Zn1-N1	2.0531(3)
Zn1-I2	2.5319(6)	Zn1-N4#1	2.0696(3)

I2-Zn1-I1	120.21(2)	N4#1-Zn1-I2	109.50(9)
N1-Zn1-I1	107.77(9)	C5-N1-Zn1	124.30(2)
N1-Zn1-I2	109.50(9)	C1-N1-Zn1	117.23(3)
N1-Zn1-N4#1	99.13(12)	C23-N4-Zn1#2	117.89(2)
N4#1-Zn1-I1	108.66(9)	C24-N4-Zn1#2	123.68(2)

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