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The effect of iodide on electronic and photo-responsive behaviors of 1D naphthalenediimide-based zinc coordination polymers

Yifang Zhang, Ming Kang, Shimin Zhang, Bohong Gao, Pengfei Hao,*

Junju Shen, Gaopeng Li and Yunlong Fu*

Key Laboratory of Magnetic Molecules & Magnetic Information Materials Ministry of Education, School of Chemical and Material Science, Shanxi Normal University, Taiyuan 030001, China

**Corresponding author. Tel: +86-13835388909.*

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

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1. Figures

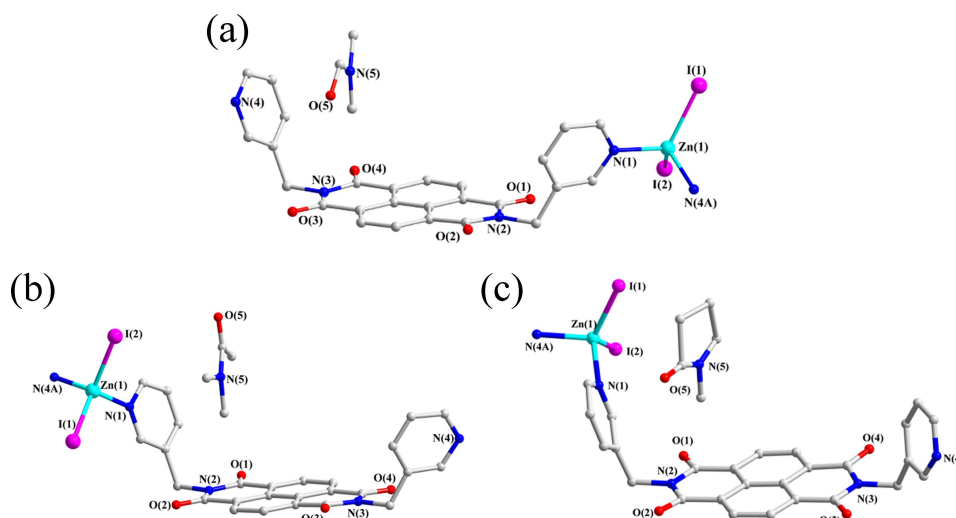


Fig. S1 (a) Coordination environment of Zn^{2+} in **2** (symmetry codes: A: $0.5+x, 0.5-y, -0.5+z$); (b) Coordination environment of Zn^{2+} in **3** (symmetry codes: A: $-0.5+x, 1.5-y, 0.5+z$); (c) Coordination environment of Zn^{2+} in **4** (symmetry codes: A: $-0.5+x, 1.5-y, 0.5+z$); All hydrogen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

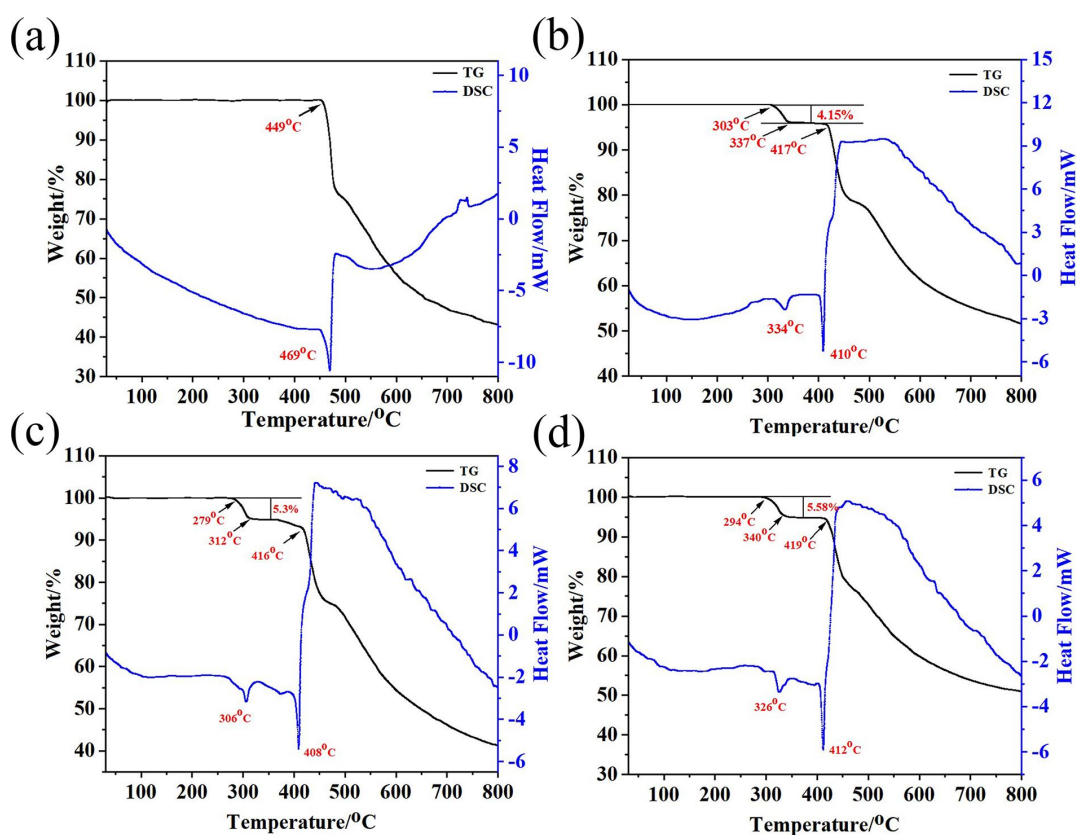


Fig. S2 Thermo-gravimetric (TG) and Differential scanning calorimetry (DSC) curves of **1-4**.

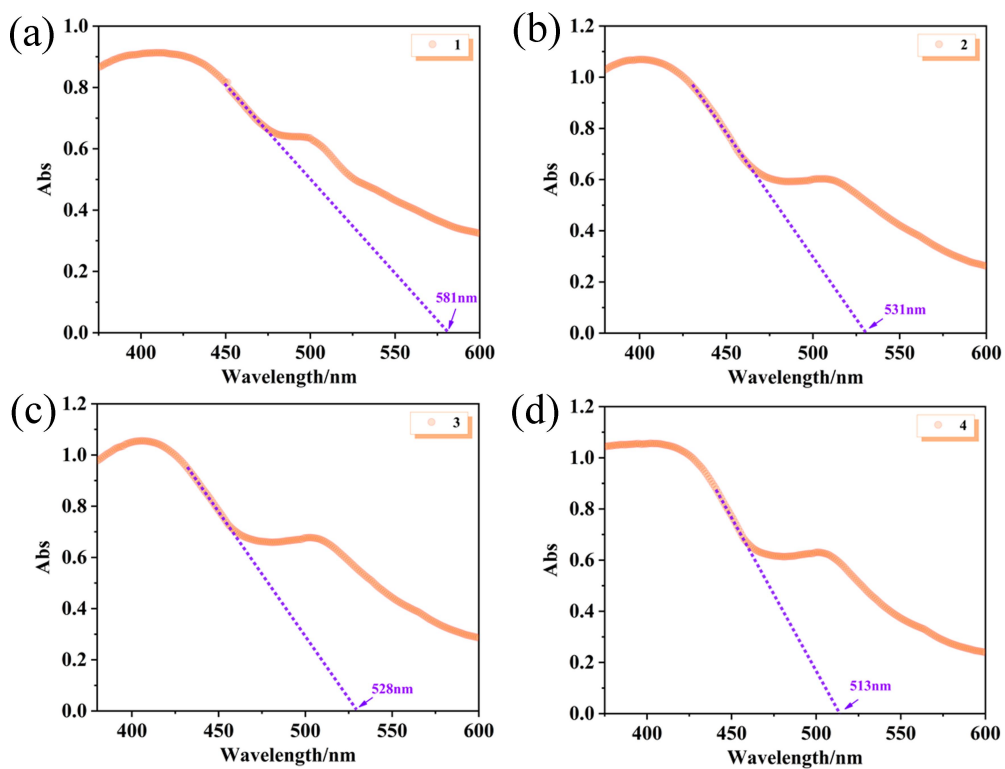


Fig. S3 Kubelka-Munk transformed reflectivity vs energy of complexes 1-4.

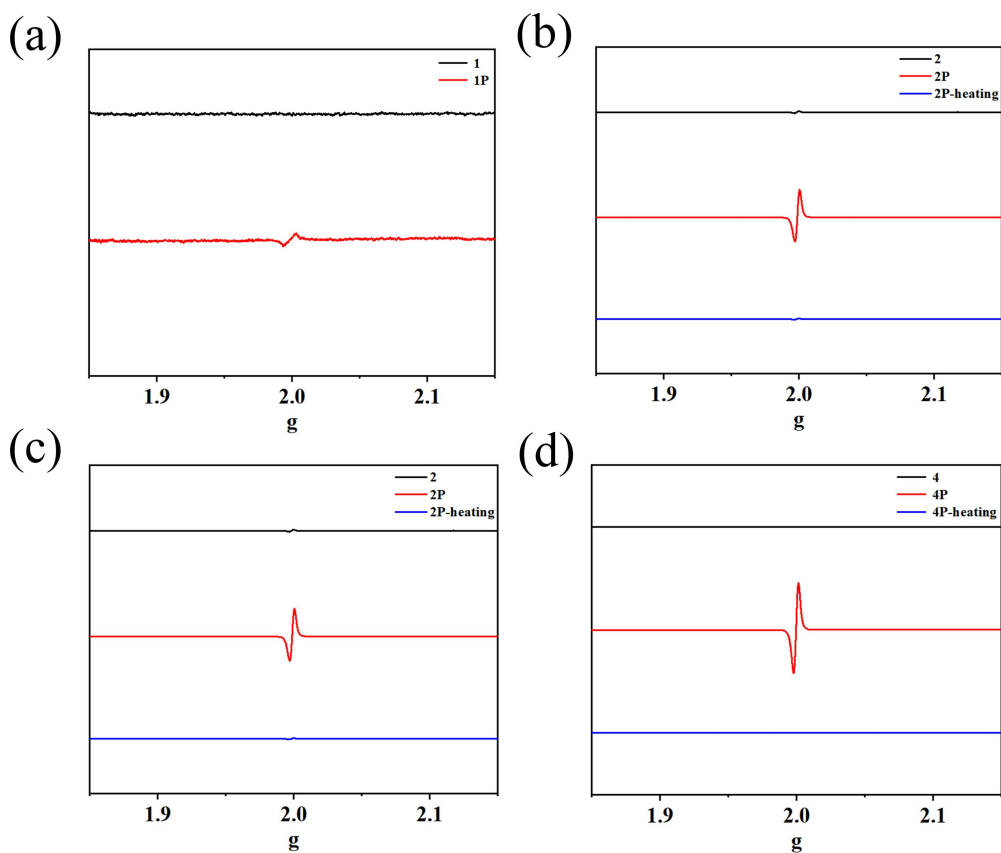


Fig. S4 The EPR spectra of 1 and 1P (a), 2, 2P and 2P-heating (b), 3, 3P and 3P-heating (c) and 4, 4P and 4P-heating (d).

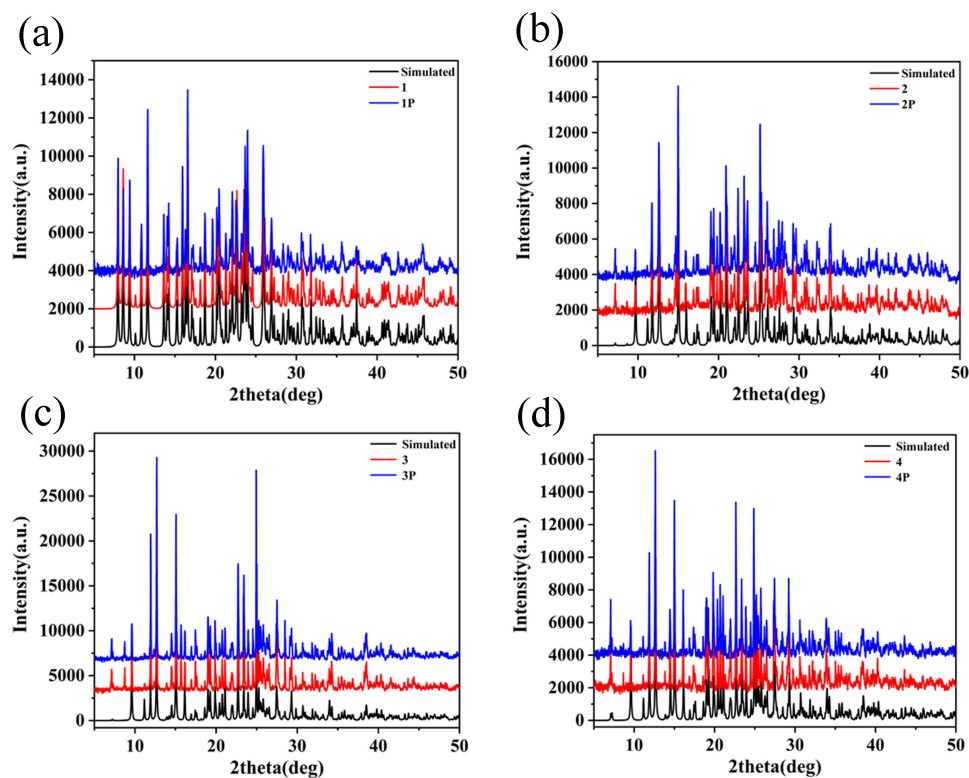


Fig. S5 PXRD patterns of **1-4** simulated from the X-ray single-crystal structures, as-synthesized samples and after irradiation samples.

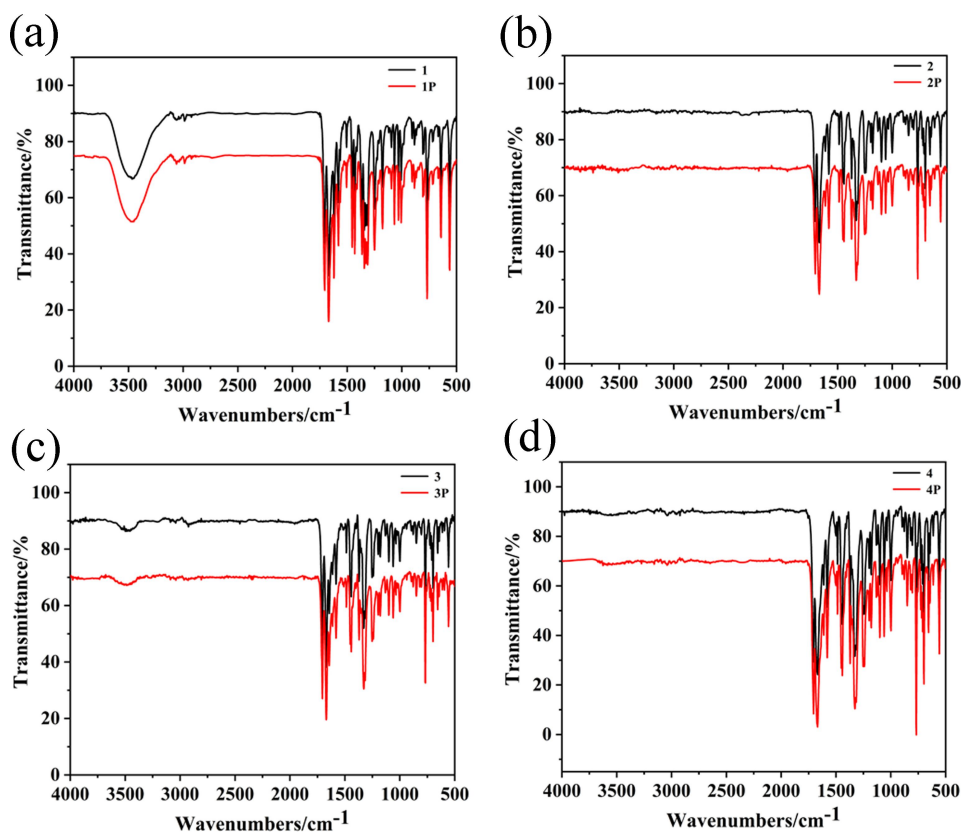


Fig. S6 FT-IR spectra of **1-4** as-synthesized samples and after irradiation samples.

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 ₂ N ₄ O ₄ Zn	C ₅₅ H ₃₉ I ₄ N ₉ O ₉ Zn ₂	C ₅₆ H ₄₁ I ₄ N ₉ O ₉ Zn ₂	C ₅₇ H ₄₁ I ₄ N ₉ O ₉ Zn ₂
Formula weight	767.60	1608.29	1622.32	1634.33
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	<i>P</i> -1	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>
<i>a</i> (Å)	10.1573(9)	25.3483(17)	25.493(4)	25.494(3)
<i>b</i> (Å)	12.2406(11)	13.9149(8)	13.949(3)	13.9506(19)
<i>c</i> (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
<i>V</i> (Å ³)	1315.6(2)	5574.5(6)	5631.9(17)	5636.0(13)
<i>Z</i>	2	4	4	4
<i>D_c</i> (g cm ⁻³)	1.938	1.916	1.913	1.926
μ (mm ⁻¹)	3.320	3.140	3.109	3.108
<i>F</i> (000)	736.0	3104.0	3136.0	3160.0
Reflections collected	21144	50128	41656	50537
Independent reflections	6510	6898	7088	6992
<i>R</i> _{int}	0.0382	0.0570	0.0471	0.0448
Goodness-of-fit on <i>F</i> ²	1.005	0.961	1.018	0.932
<i>R</i> ₁ / <i>wR</i> ₂ , [<i>I</i> ≥ 2σ(<i>I</i>)] ^{a,b}	0.0465/0.0805	0.0445/0.1268	0.0426/0.0825	0.0373/0.1142
<i>R</i> ₁ / <i>wR</i> 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 $1/2+x, 3/2-y, -1/2+z$
