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Reversible luminescence tuning behavior in a thermal-stimuli-responsive anthracene-based coordination polymer

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A. Supporting Figures.

Fig. S1 The two-dimensional sheet of **HPU-22**.

Fig. S2 The three-dimensional framework of **HPU-22**, mediated by intermolecular O2···H9A-O9, O12···H9B-O9, O12···H11-O11 interactions.

Fig. S3 The SEM image and elemental mapping of **HPU-22**.

Fig. S4 The XRD patterns of simulated **HPU-22** and synthesized **HPU-22**.

Fig. S5 The state diagram of **HPU-22** after grinding.

Fig. S6 The PXRD patterns of **HPU-22** and **HPU-22** heating at different temperatures.

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Fig. S8 The performance of **HPU-22H200** with adding different solvents under UV light (1. Water; 2. CH_3OH; 3. CH_3CH_2OH; 4. DMA; 5. DMF; 6. CH_3CN).

B. Supporting Tables

Table S1 Crystal data and structure refinement for complexes **HPU-22** and **HPU-22H200**.

Table S2 Selected bond distances /Å and bond angles /° for **HPU-22** and **HPU-22H200**.

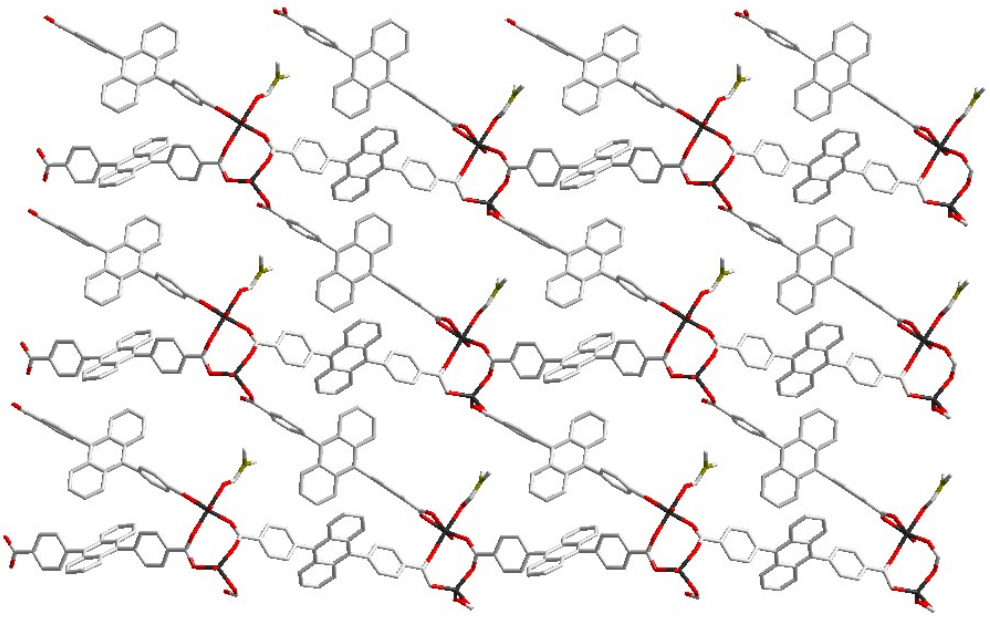

Fig. S1 The two-dimensional sheet of **HPU-22**.

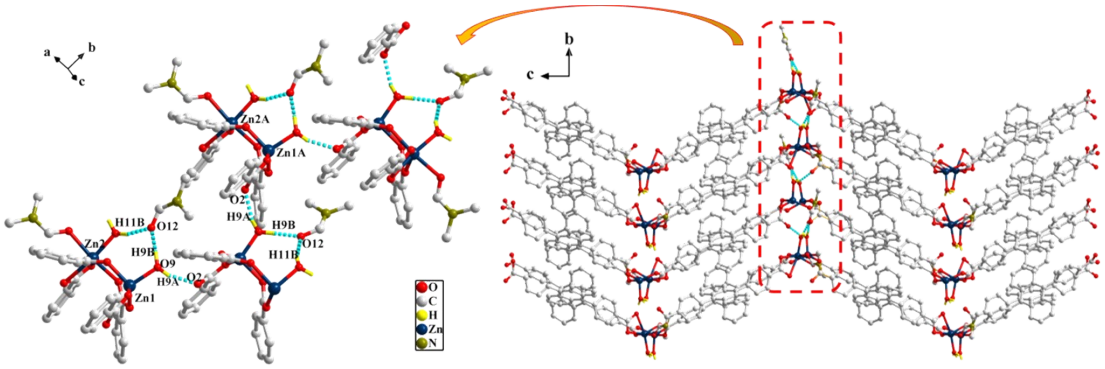

Fig. S2 The three-dimensional framework of **HPU-22**, mediated by intermolecular O2···H9A-O9, O12···H9B-O9, O12···H11-O11 interactions.

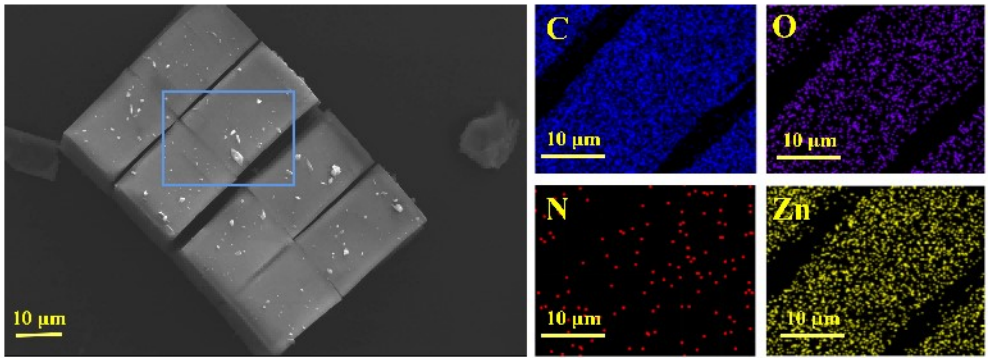

Fig. S3 The SEM image and elemental mapping of **HPU-22**.

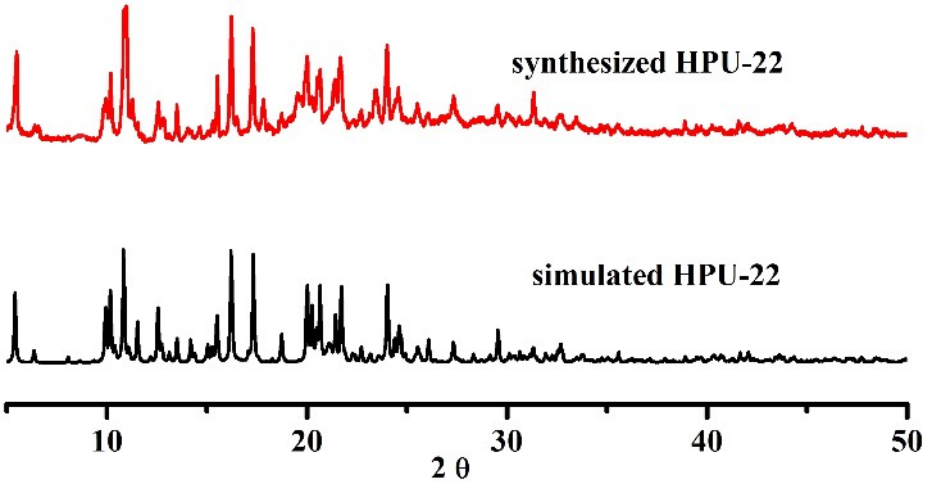

Fig. S4 The XRD patterns of simulated **HPU-22** and synthesized **HPU-22**.

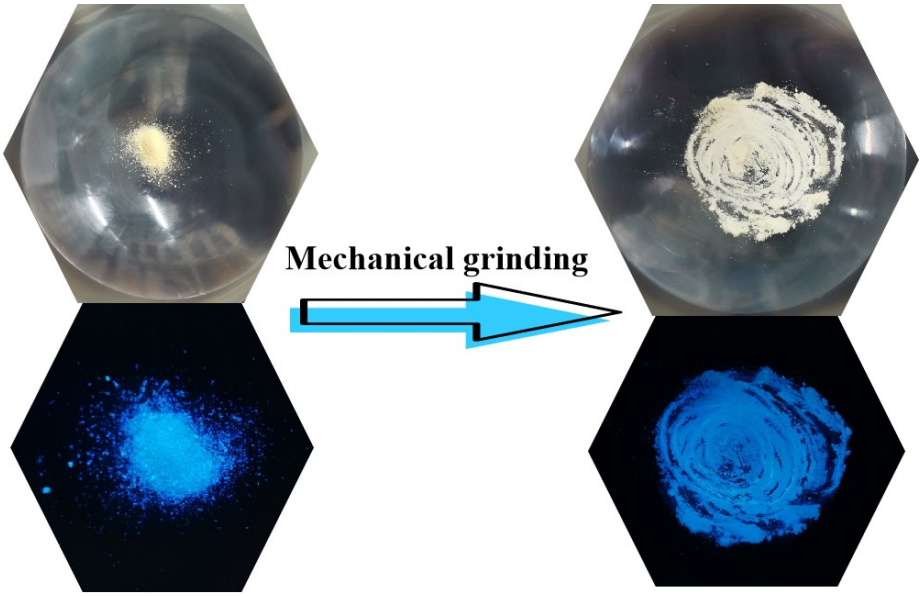

Fig. S5 The state diagram of **HPU-22** after grinding.

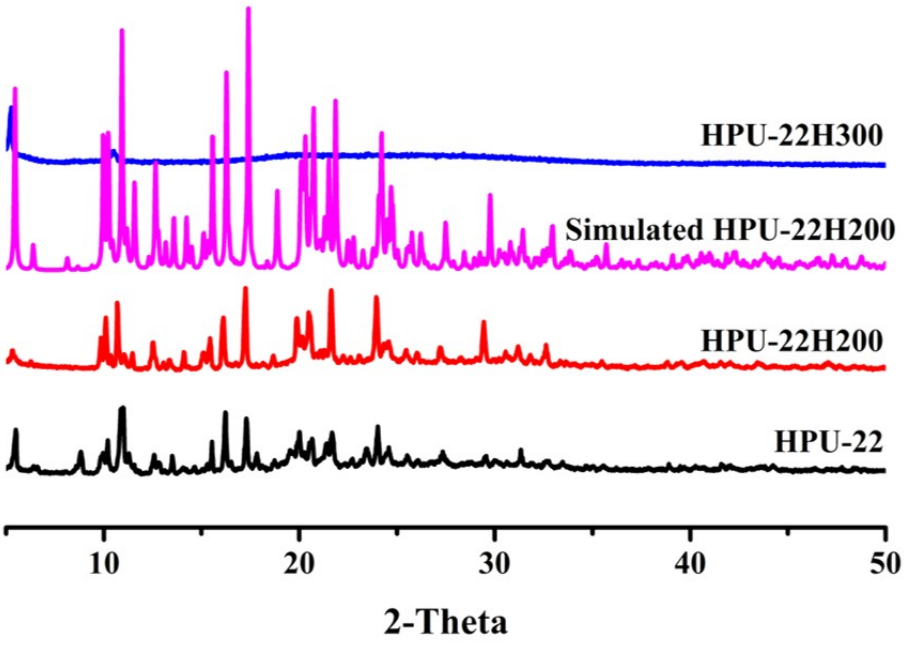

Fig. S6 The PXRD patterns of **HPU-22** and **HPU-22** heating at different temperatures.

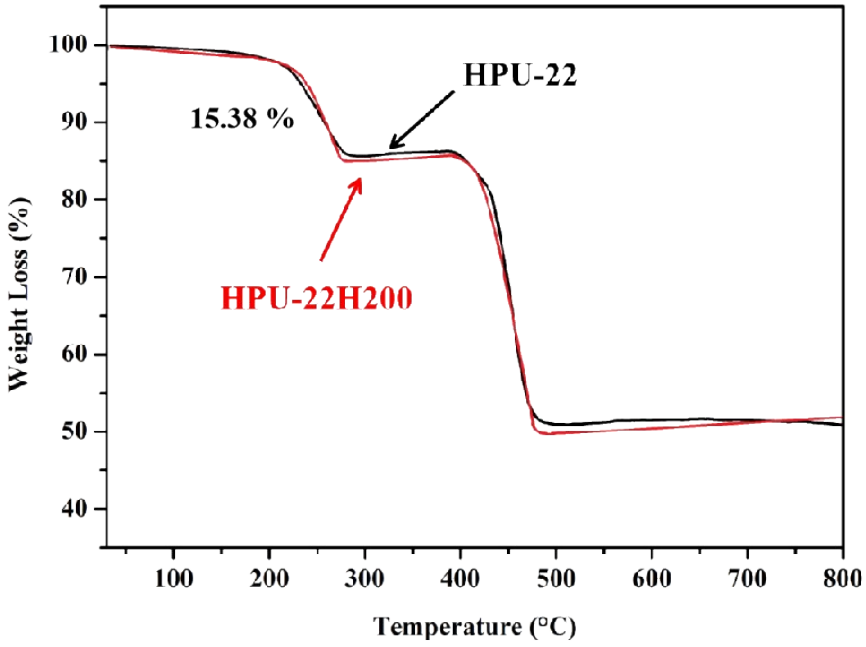

Fig. S7 The TG results of **HPU-22** and **HPU-22H200**.

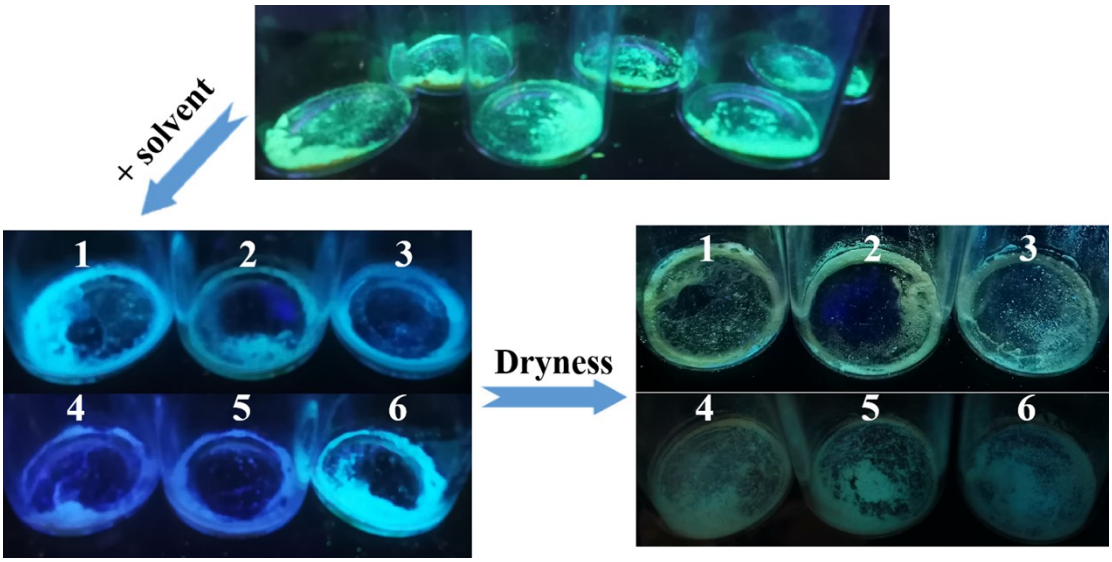

Fig. S8 The performance of **HPU-22H300** with adding different solvents under UV light. (1. Water; 2. CH_3OH; 3. CH_2CH_2OH; 4. DMA; 5. DMF; 6. CH_3CN)

Table S1 Crystal data and structure refinement for complexes **HPU-22** and **HPU-22H200**[ab]

Compound	**HPU-22**	**HPU-22H200**
Formula	$C_{62}H_{50}N_2O_{12}Zn_2$	$C_{62}H_{50}N_2O_{12}Zn_2$
fw	1145.78	1145.78
T/K	293(2)	296(2)
λ (Mo Kα), Å	0.71073	0.71073
cryst syst	*monoclinic*	*Monoclinic*
space group	*P 21/c*	*P 21/c*
a/Å	13.9085(3)	13.8555(3)
b/Å	11.5933(6)	11.5530(3)
c/Å	32.6997(9)	32.4314(8)
α/deg	90	90
β/deg	93.957(2)	93.670(1)
γ/deg	90	90
V/Å^3	5260.1(3)	5180.7(2)
Z	4	4
$D_{calcd.}$(g·cm^{-3})	1.447	1.469
F(000)	2368.0	2368.0
$2\theta_{max}$(º)	25.00	27.461
GOF	1.028	1.042
R_1(I>2sigma(I))[a]	0.0451	0.0457
wR_2 (all data)[b]	0.1094	0.1035

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

Table S2 Selected bond distances /Å and bond angles /° for **HPU-22** and **HPU-22H200**.

HPU-22			
Zn1-O7	1.924(2)	O1-Zn1-O9	103.45(9)
Zn1-O9	1.988(2)	O1-Zn1-O5	102.07(9)
Zn1-O5	1.947(2)	O11-Zn2-O8^{iii}	89.27(8)
Zn1-O1	1.945(2)	O11-Zn2-O10	84.06(9)
Zn2-O6	1.993(2)	O3^{iv}-Zn2-O4^{iv}	58.01(9)
Zn2-O10	2.192(2)	O3^{iv}-Zn2-O8^{iii}	93.25(8)
Zn2-O11	2.018(2)	O3^{iv}-Zn2-O10	89.13(9)
Zn2^{ii}-O8	2.1091(19)	O8^{iii}-Zn2-O10	173.29(9)
Zn2^{i}-O3	2.048(2)	O6-Zn2-O4^{iv}	88.38(9)
O7^{iii}-Zn1-O9	110.35(10)	O6-Zn2-O3^{iv}	146.25(10)
O7^{iii}-Zn1-O5	118.46(9)	O6-Zn2-O10	85.43(9)
O7^{iii}-Zn1-O1	119.48(9)	O11-Zn2-O4^{iv}	159.99(8)
O5-Zn1-O9	100.47(9)	O11-Zn2-O3^{iv}	104.30(10)
HPU-22H200			
Zn1-O1^{i}	2.1097(19)	O12-Zn1-O1^{i}	89.37(8)
Zn1-O8	1.9914(18)	O8-Zn1-O7^{ii}	147.05(8)
Zn1-O12	2.012(2)	O8-Zn1-O2	85.41(8)
Zn1-O7^{ii}	2.059(2)	O12-Zn1-O7^{ii}	103.45(9)
Zn1-O2	2.187(2)	O12-Zn1-O2	84.67(8)
Zn2-O4	1.9290(19)	O7^{ii}-Zn1-O1^{i}	93.58(8)
Zn2-O6	1.9463(19)	O7^{ii}-Zn1-O2	88.78(8)
Zn2-O10^{iii}	1.9461(19)	O4-Zn2-O6	119.07(9)
Zn2-O9	1.9878(19)	O4-Zn2-O10^{iii}	117.81(9)
O8-Zn1-O12	108.23(9)	O4-Zn2-O9	110.82(9)
O1^{i}-Zn1-O2	173.96(8)	O6-Zn2-O9	103.54(9)
O1^{i}-Zn1-O11^{ii}	99.72(7)	O10^{iii}-Zn2-O6	102.72(8)
O8-Zn1-O1^{i}	95.55(8)	O10^{iii}-Zn2-O9	100.45(8)

Symmetry operations for **HPU-22**: (i) -1+x, 1.5-y, -0.5+z; (ii) x, 1.5-y, -0.5+z; (iii) x, 1.5-y, 0.5+z; (iv) 1+x, 1.5-y, 0.5+z.

Symmetry operations for **HPU-22H200**: (i) x, 0.5-y, -0.5+z; (ii) -1+x, y, -1+z; (iii) x, 0.5-y, 0.5+z; (iv) 1+x, y, 1+z.