

Supporting Information

Two 2D multiresponsive luminescence coordination polymers for selective sensing of Fe³⁺, Cr^{VI}-anions and TNP in aqueous medium

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Table S1 Selected bond lengths (Å) and angles (°) for **1** and **2**.

CP 1			
Zn1-O4A	1.920(4)	Zn1-O7	2.237(5)
Zn1-O1	1.931(4)	Zn1-O6	2.258(4)
Zn1-N2B	2.045(4)		
O4A-Zn1-O1	127.43(16)	N2B-Zn1-O7	90.37(18)
O4A-Zn1-N2B	128.81(17)	O4A-Zn1-O6	90.13(17)
O1-Zn1-N2B	103.75(17)	O1-Zn1-O6	90.35(17)
O4A-Zn1-O7	91.41(18)	N2B-Zn1-O6	88.93(17)
O1-Zn1-O7	88.44(18)	O7-Zn1-O6	178.42(15)
Symmetry codes: A -x+1, y+1/2, -z+3/2; B -x+2, -y+1, -z+2.			
CP 2			
Cd1-O6	2.249(12)	Cd1-O1B	2.474(9)
Cd1-O7	2.273(12)	Cd1-O3	2.667(9)
Cd1-O4	2.302(9)	N2-Cd1C	2.318(11)
Cd1-N2A	2.318(11)	O2-Cd1D	2.377(10)
Cd1-O2B	2.377(10)		
O6-Cd1-O7	171.9(4)	O7-Cd1-O4	88.7(4)
O6-Cd1-O4	97.8(4)	O6-Cd1-N2A	83.4(4)
O7-Cd1-N2A	88.5(5)	O4-Cd1-N2A	138.1(3)

O6-Cd1-O2B	92.3(4)	O7-Cd1-O2B	93.5(4)
O4-Cd1-O2B	81.6(3)	N2A-Cd1-O2B	140.3(4)
O6-Cd1-O1B	92.4(4)	O7-Cd1-O1B	86.4(4)
O4-Cd1-O1B	134.8(3)	N2A-Cd1-O1B	86.6(3)
O2B-Cd1-O1B	54.0(3)	O6-Cd1-O3	90.9(4)
O7-Cd1-O3	89.1(4)	O4-Cd1-O3	52.5(3)
N2A-Cd1-O3	85.7(3)	O2B-Cd1-O3	134.0(3)
O1B-Cd1-O3	171.2(3)		

Symmetry codes: A -x+1, y+1/2, -z+3/2; B -x+2, -y+1, -z+2.

Table S2 Hydrogen bond lengths (Å) and angles (°) for CP **1**^a.

D	A[Transformation]	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O6	O3[-x+1, -y+1, -z+1]	0.850	1.940	2.788	176(2)
O6	O2[-x+1, -y+2, -z+1]	0.850	1.923	2.749	164(2)
O7	O5[-x+1, -y+2, -z]	0.850	1.948	2.780	166(3)
O7	O8	0.850	2.353	2.989	153(3)
O8	O6[x-1, y, z]	0.850	2.095	2.931	168(2)

^aD, donor; A, acceptor.

Table S3 Hydrogen bond lengths (Å) and angles (°) for CP **2**^a.

D	A[Transformation]	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O6	O3[-x+1, -y+1, -z+2]	0.850	1.869	2.718	177.30
O6	O9	0.850	2.097	2.943	173.19
O7	O1[-x, -y+1, -z+2]	0.850	1.924	2.751	163.95
O8	O11[x, y+1, z]	0.850	2.008	2.858	178.51
O9	O10[x+1, y+1, z]	0.850	2.039	2.839	156.41
O9	O11[x, y+1, z]	0.850	1.871	2.666	155.05
O10	O2	0.850	2.057	2.907	179.78
O10	O5 [-x, -y+1, -z+1]	0.850	2.062	2.911	179.52
O11	O8[-x+1, -y+1, -z+1]	0.850	2.323	3.127	157.85
O11	O10[-x+1, -y, -z+1]	0.850	1.981	2.779	155.89

N1	O8[-x+1, -y+1, -z+1]	0.860	2.053	2.893	165.51
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^aD, donor; A, acceptor.

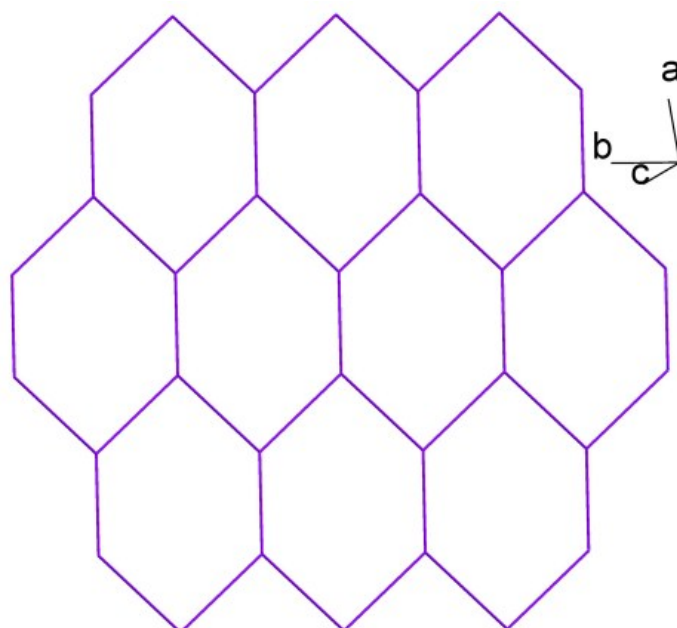


Fig. S1 The schematic view of the hcb topology of the 2D layer.

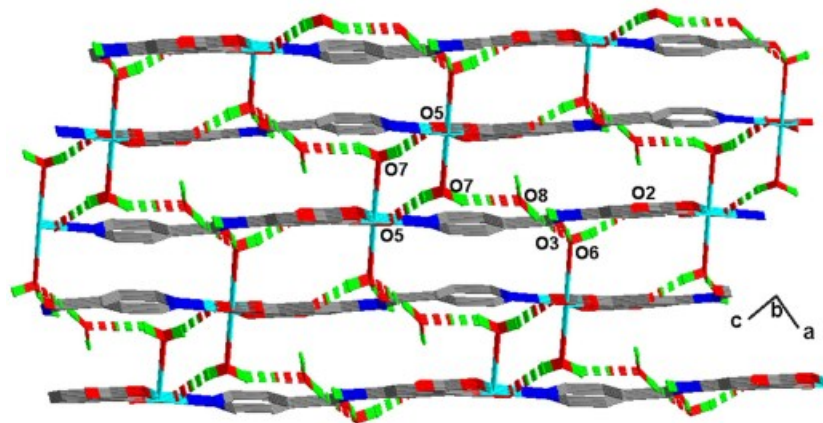


Fig. S2 The 3D packing of the layers in **1**.

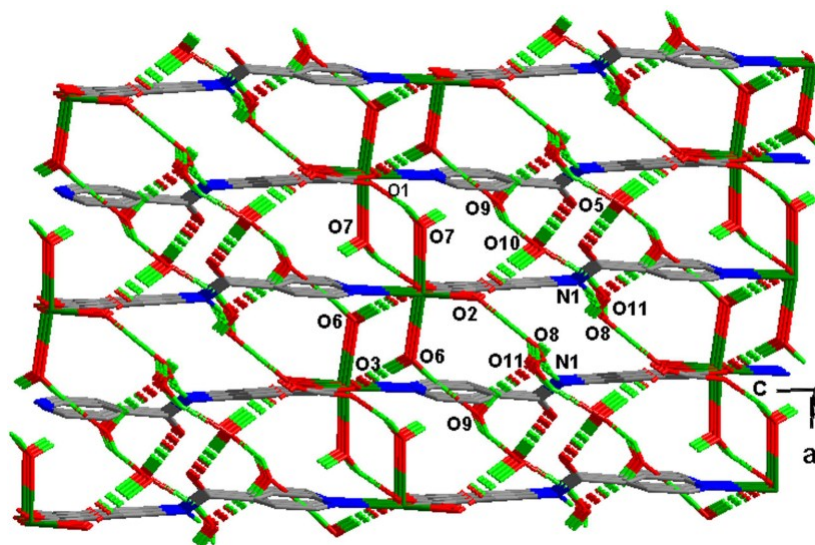


Fig. S3 The 3D packing of the layers in **2**.

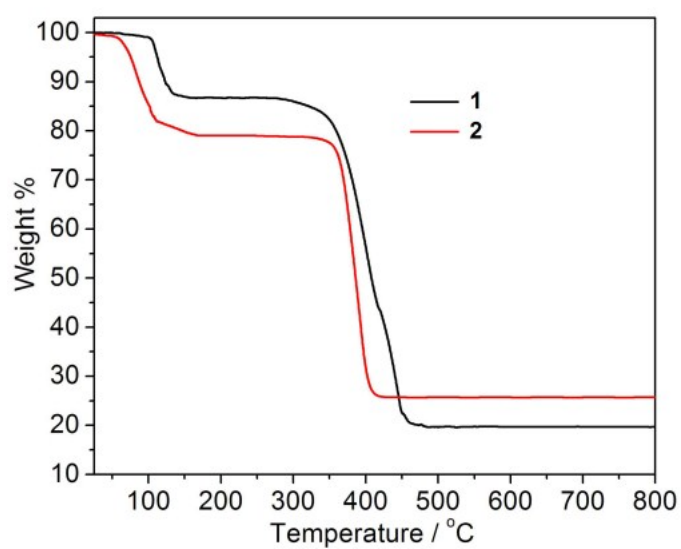


Fig. S4 TGA curves of **1** and **2**.

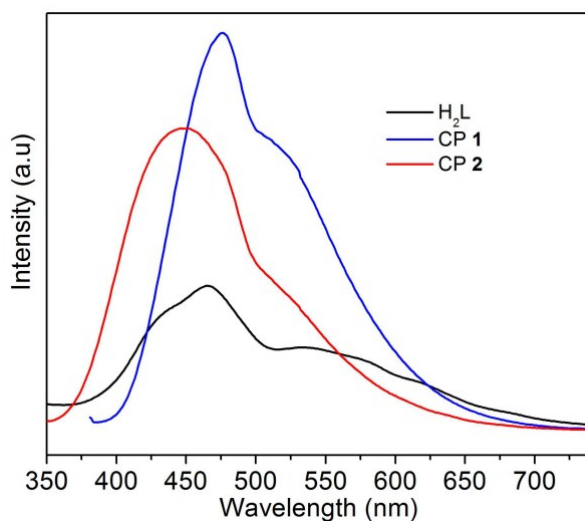


Fig. S5 The solid-state emission spectra of free H_2L , **1** and **2** at room temperature.

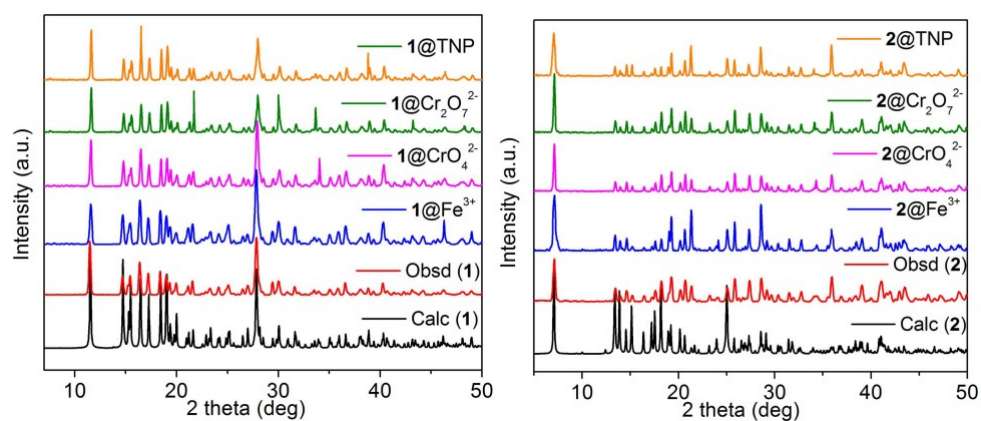


Fig. S6 The powder X-ray diffraction patterns of simulated **1** and **2**, as-synthesized **1** and **2** and CPs **1** and **2** immersed in 1.0 mM water solutions of Fe^{3+} , CrO_4^{2-} , $\text{Cr}_2\text{O}_7^{2-}$ and TNP.

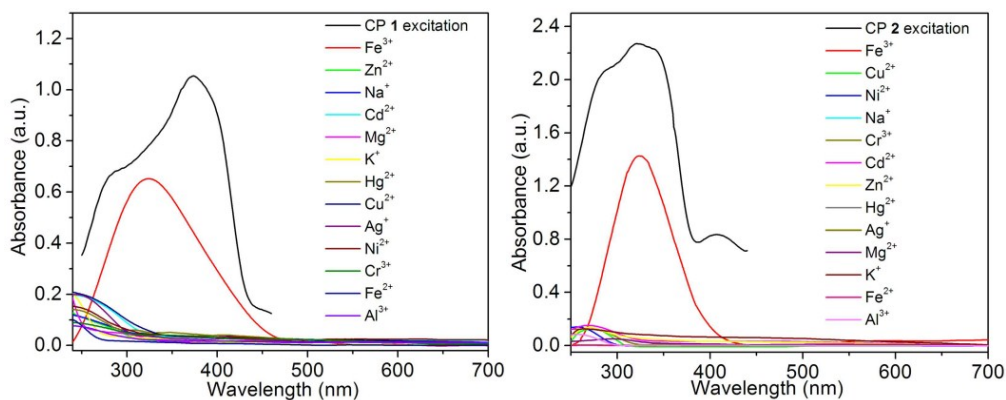


Fig. S7 The UV-Vis absorption spectra of **1** and **2** immersed in different metal ions aqueous solution and the corresponding excitation for **1** and **2**.

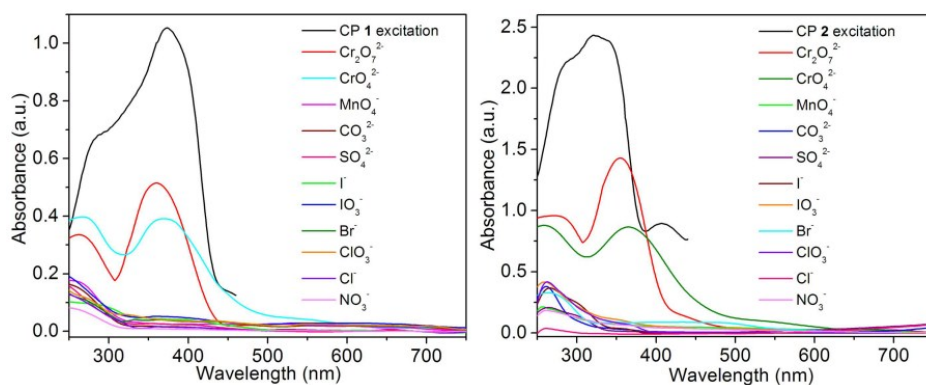


Fig. S8 The UV-Vis absorption spectra of **1** and **2** immersed in different anions aqueous solution and the corresponding excitation for **1** and **2**.

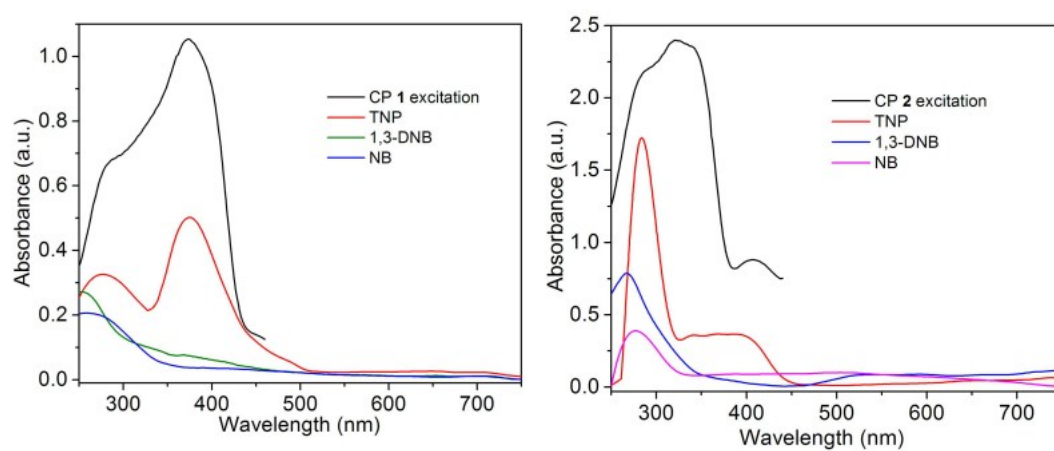


Fig. S9 The UV-Vis absorption spectra of **1** and **2** immersed in NB, 1,3-DNB and TNP aqueous solution, and the corresponding excitation for **1** and **2**.