

Multifunctional polymers with interpenetrating structures: luminescent sensing, ECL behaviors, selective detection of Fe³⁺ ion and rapid removal of anionic dyes

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Table S1 Crystal and Structure Refinement Data for Compounds 1-3

Compound	1	2	3
CCDC No.	1978114	1978115	1978117
Formula	C ₅₀ H ₄₄ Cd ₂ N ₁₀ O ₁₆	C ₆₈ H ₆₆ N ₁₂ O ₁₁ Zn ₂	C ₆₄ H ₅₄ N ₁₀ O ₁₅ Zn ₂
Fw	1265.75	1358.07	1333.91
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	<i>Ia</i>	<i>C2/c</i>	<i>Pbcn</i>
a/Å	18.3533(9)	22.4550(10)	23.392(4)
b/Å	6.6978(3)	13.5382(6)	11.662(2)
c/Å	28.1756	24.5285(10)	27.060(5)
α(°)	90.00	90.00	90.00
β(°)	95.0010(10)	112.0620(10)	90.00
γ(°)	90.00	90.00	90.00
V(Å ³)	3450.3(3)	6910.7(5)	7382(2)
Z	2	4	4
Dc(g cm ⁻³)	1.218	1.305	1.200
μ/mm ⁻¹	0.677	0.760	0.714
F(000)	1276	2824	2752
GOF on F ²	1.129	1.069	1.183
R ₁ /wR ₂ [I>2σ(I)]	0.0529, 0.1506	0.0718, 0.2190	0.0975, 0.2779
R ₁ /wR ₂ (all data)	0.0675, 0.1647	0.0998, 0.2518	0.1755, 0.3464

Table S2.Selected Bond Lengths (Å) and Angles (deg) for Compounds 1-3

Compound 1			
N(5)-Cd(1)#2	2.258(11)	O(1)-Cd(1)#1	2.306(8)
O(2)-Cd(1)#1	2.470(13)	O(3)-Cd(1)	2.396(10)
O(4)-Cd(1)	2.290(11)	Cd(1)-N(5)#3	2.258(11)
O(1)-Cd(1)#1	2.306(8)	O(2)-Cd(1)#1	2.470(13)
O(3)-Cd(1)	2.396(10)	O(4)-Cd(1)	2.290(11)
Cd(1)-N(5)#3	2.258(11)	Cd(1)-O(1)#4	2.306(8)
Cd(1)-O(2)#4	2.470(13)	N(2)-Cd(1)	2.238(11)
N(2)-Cd(1)-N(5)#3	105.50(18)	N(2)-Cd(1)-O(4)	97.7(4)
N(5)#3-Cd(1)-O(4)	140.3(4)	N(2)-Cd(1)-O(1)#4	140.8(4)
N(5)#3-Cd(1)-O(1)#4	94.6(4)	O(4)-Cd(1)-O(1)#4	86.7(2)
N(2)-Cd(1)-O(3)	91.2(4)	N(5)#3-Cd(1)-O(3)	95.2(4)
O(4)-Cd(1)-O(3)	52.0(4)	O(1)#4-Cd(1)-O(3)	120.6(4)
N(2)-Cd(1)-O(2)#4	89.7(4)	N(5)#3-Cd(1)-O(2)#4	90.5(4)
O(4)-Cd(1)-O(2)#4	121.7(4)	O(3)-Cd(1)-O(2)#4	173.8(3)
Symmetry codes: #1 x,-y-1/2,z-1/2 #2 x+1/2,-y+2,z #3 x-1/2,-y+2,z #4 x,-y-1/2,z+1/2			
Compound 2			
Zn(1)-O(1)	1.938(3)	Zn(1)-N(2)	2.026(3)
Zn(1)-N(5)#1	2.035(3)	Zn(1)-O(3)#2	2.049(7)
N(5)-Zn(1)#3	2.035(3)	O(3)-Zn(1)#4	2.049(7)
O(1)-Zn(1)-N(2)	111.09(16)	O(1)-Zn(1)-N(5)#1	112.99(14)
N(2)-Zn(1)-N(5)#1	102.04(13)	O(1)-Zn(1)-O(3)#2	95.7(2)
N(2)-Zn(1)-O(3)#2	136.5(3)	N(5)#1-Zn(1)-O(3)#2	97.8(2)
C(1)-O(1)-Zn(1)	116.8(3)	C(29)-N(5)-Zn(1)#3	126.1(3)
C(30)-N(5)-Zn(1)#3	127.6(3)	C(16)-N(2)-Zn(1)	127.3(3)
C(14)-N(2)-Zn(1)	125.7(3)	C(13)-O(3)-Zn(1)#4	100.5(7)
Symmetry codes: #1 x+1/2,-y-1/2,z+1/2 #2 x,-y+1,z-1/2 #3 x-1/2,-y-1/2,z-1/2 #4 x,-y+1,z+1/2			
Compound 3			
N(2)-Zn(1)	2.010(4)	N(5)-Zn(1)#1	2.005(4)
O(1)-Zn(1)	1.926(4)	O(4)-Zn(1)#2	1.968(3)
Zn(1)-O(4)#4	1.968(3)	Zn(1)-N(5)#5	2.005(4)
O(1)-Zn(1)-O(4)#4	96.68(14)	O(1)-Zn(1)-N(5)#5	109.05(17)
O(4)#4-Zn(1)-N(5)#5	110.31(14)	O(1)-Zn(1)-N(2)	117.16(17)
O(4)#4-Zn(1)-N(2)	107.05(14)	N(5)#5-Zn(1)-N(2)	114.94(16)
Symmetry codes: #1 x-1/2,-y-3/2,-z+1 #2 x,-y,z-1/2 #3 -x,y,-z+1/2 #4 x,-y,z+1/2 #5 x+1/2,-y-3/2,-z+1			

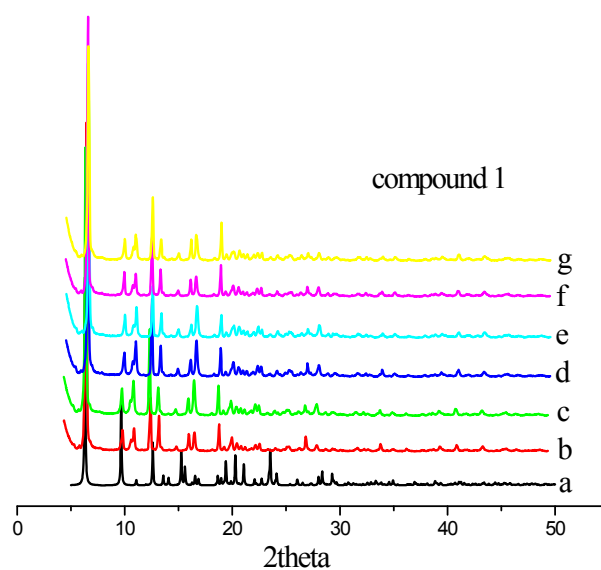


Figure S1. Simulated (a), as-synthesized (b), immersed in water after 2 days (c), immersed in PBS solution (0.1M, PH=11) after 2 days (d), immersed in Fe³⁺ (0.01M) after 2 days (e), after releasing test for CR (f), and vacuuming at 80°C for 12 hours (g) powder X-ray diffraction patterns of **1**.

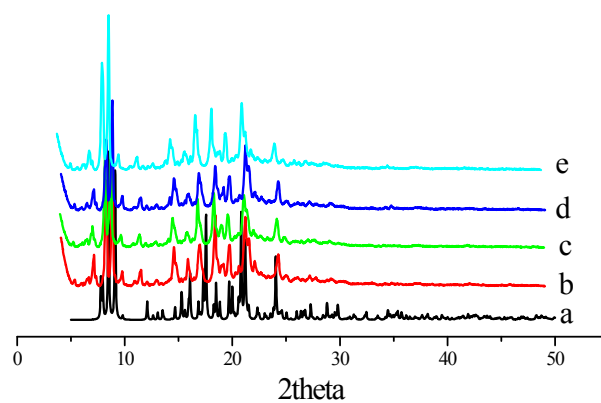


Figure S2. Simulated (a), as-synthesized (b), immersed in PBS solution (0.1M, PH=11) after 2 days (c), after releasing test for MO (d), and vacuuming at 80°C for 12 hours (e) powder X-ray diffraction patterns of **2**.

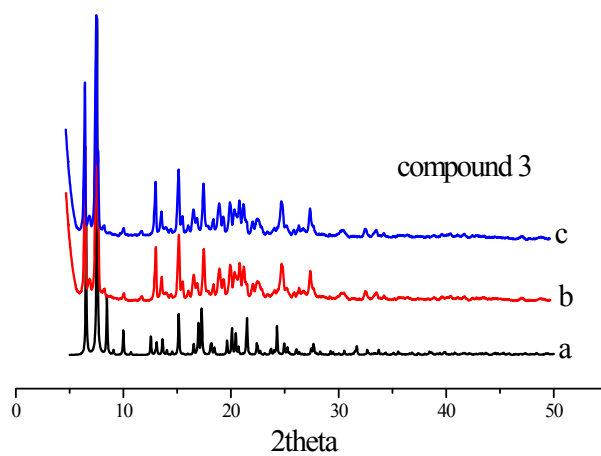


Figure S3. Simulated (a), as-synthesized (b), immersed in PBS solution (0.1M, PH=11) after 2 days (c) powder X-ray diffraction patterns of **3**.

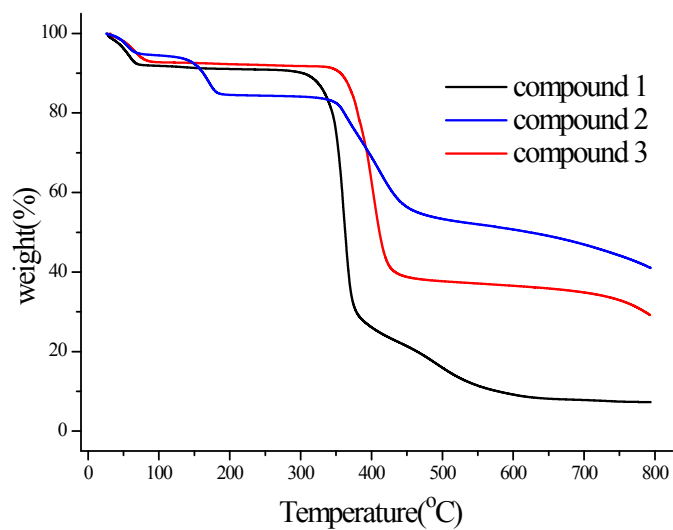


Figure S4 The TGA diagrams of compounds **1-3**.

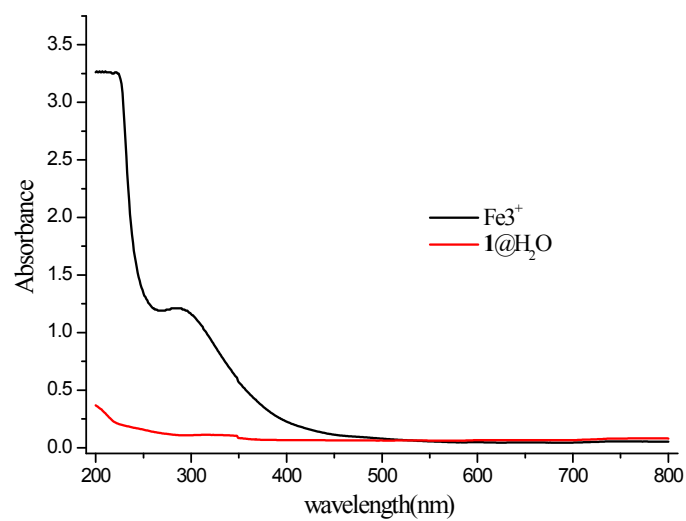


Figure S5 UV-Vis spectra of Fe³⁺, compound **1** in aqueous solution

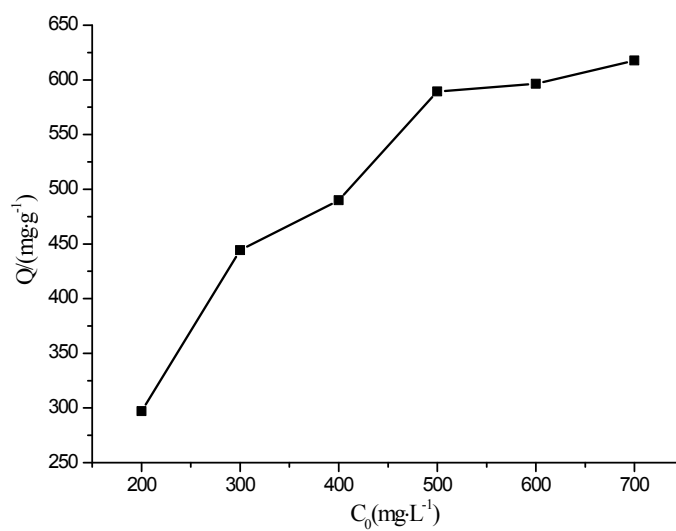


Figure S6. Adsorption isotherms for CR adsorption over 2h (compound **1**), C₀: the initial concentration of adsorbate, Q: the amount of CR adsorbed.

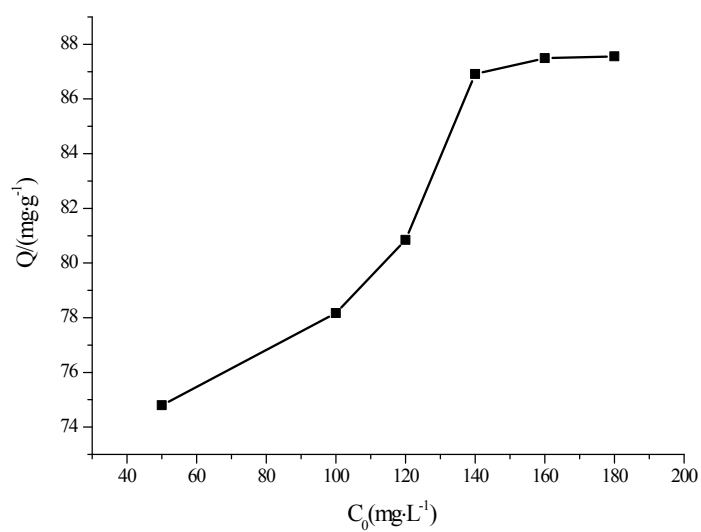


Figure S7. Adsorption isotherms for MO adsorption over 2h (compound **2**), C_0 : the initial concentration of adsorbate, Q : the amount of MO adsorbed.

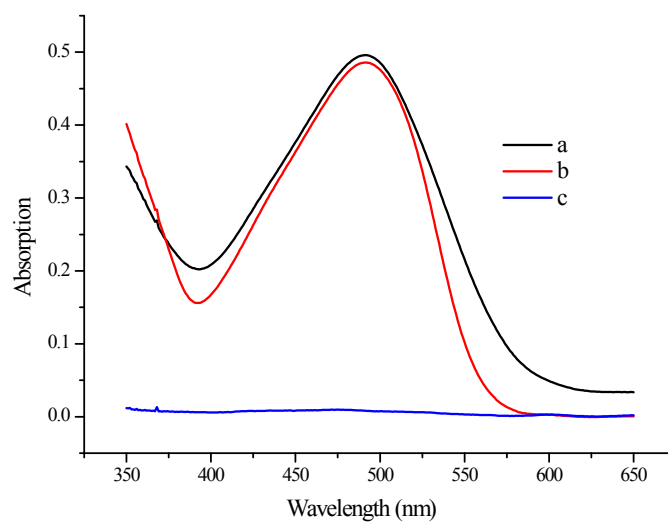


Figure S8. adsorption-desorption curve for CR (a. 5×10^{-5} CR b. **1**@CR for 30 min c. desorption for **1** by methanol)

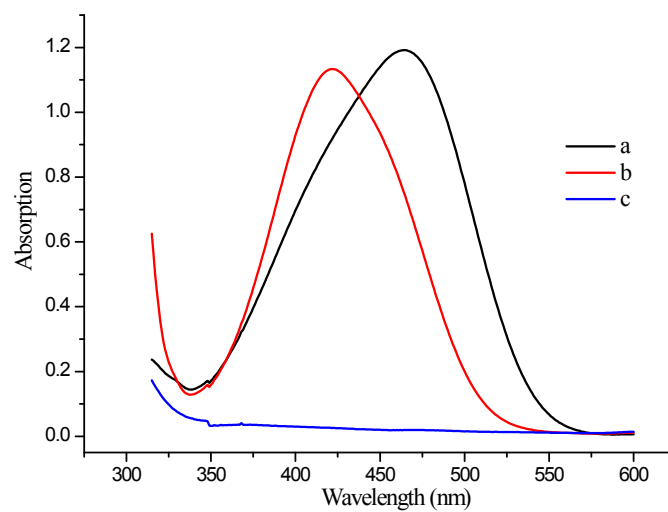


Figure S9. adsorption-desorption curve for MO (a. 5×10^{-5} CR b. **2**@CR for 30 min c. desorption for **2** by methanol)

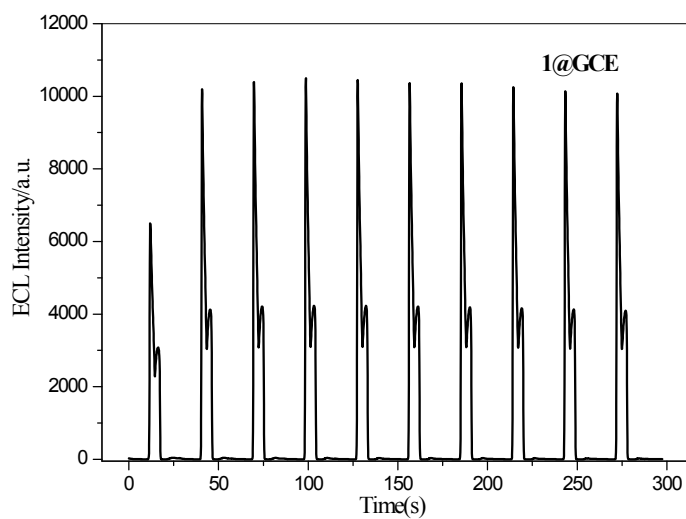


Figure S10. ECL of **1**@GCE in 0.1M PBS buffer (pH=11) and 25 mM luminol solution (ten cycles)

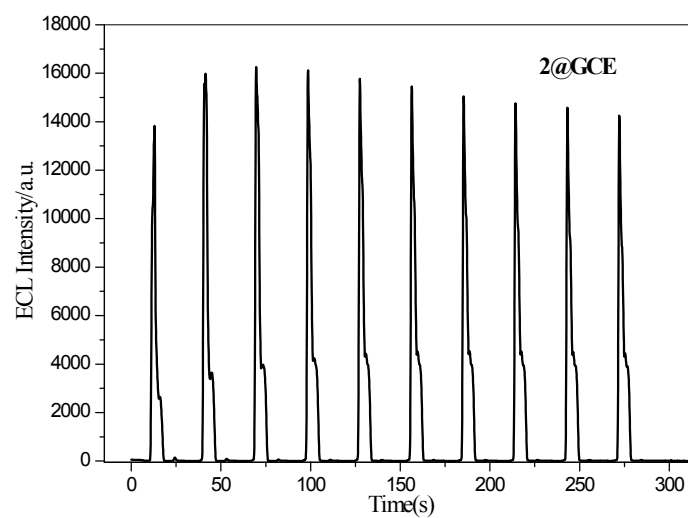


Figure S11. ECL of **2@GCE** in 0.1M PBS buffer (pH=11) and 25 mM luminol solution (ten cycles)

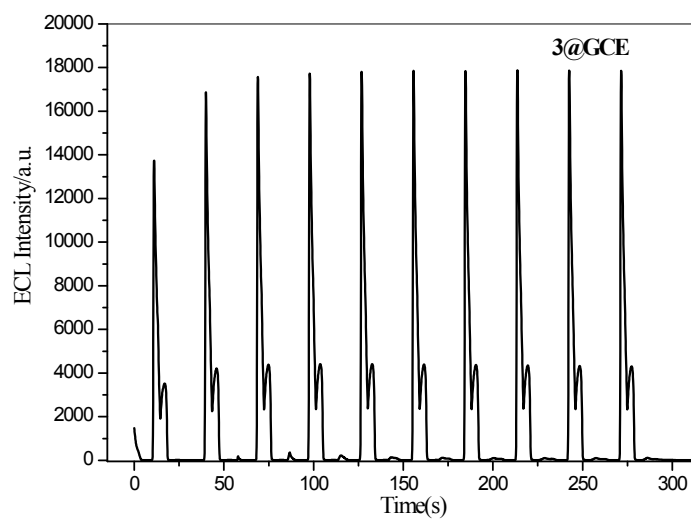


Figure S12. ECL of **3@GCE** in 0.1M PBS buffer (pH=11) and 25 mM luminol solution (ten cycles)