

# Electronic supplementary materials

## Highly selective sensing of Fe<sup>3+</sup>/Hg<sup>2+</sup> and proton conduction using two fluorescent Zn(II) coordination polymers

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**Table S1.** Selected Bond lengths [Å] and angles [°] for polymer **1** and **2**.

Polymer 1			
Zn1—O1	1.9635 (18)	Zn1—N1	2.007 (2)
Zn1—O4 <sup>i</sup>	1.9852 (19)	Zn1—N4 <sup>ii</sup>	1.998 (2)
O1—Zn1—O4 <sup>i</sup>	108.43 (8)	O4 <sup>i</sup> —Zn1—N4 <sup>ii</sup>	103.37 (8)
O1—Zn1—N4 <sup>ii</sup>	122.61 (8)	O4 <sup>i</sup> —Zn1—N1	112.60 (8)
O1—Zn1—N1	100.80 (8)	N4 <sup>ii</sup> —Zn1—N1	109.29 (9)
Polymer 2			
Zn1—O9	1.969 (2)	Zn3—N1	1.988 (3)
Zn1—O	2.079 (2)	Zn3—N12 <sup>ii</sup>	2.025 (3)
Zn1—O1	2.075 (2)	Zn3—N4 <sup>iii</sup>	1.995 (3)
Zn1—O3	1.966 (2)	Zn2—O10	1.966 (3)
Zn1—N8 <sup>i</sup>	2.048 (3)	Zn2—O8 <sup>iv</sup>	1.963 (2)
Zn3—O2	1.992 (3)	Zn2—N9	1.998 (3)
Zn3—N5	1.996 (3)		
O9—Zn1—O7	87.30 (9)	O2—Zn3—N12 <sup>ii</sup>	105.71 (11)
O9—Zn1—O1	88.38(10)	O2—Zn3—N4 <sup>iii</sup>	104.59 (13)
O9—Zn1—N8 <sup>i</sup>	116.90 (12)	N1—Zn3—O2	111.14 (12)
O1—Zn1—O7	168.39 (10)	N1—Zn3—N12 <sup>ii</sup>	106.35 (12)
O3—Zn1—O9	136.69 (11)	N1—Zn3—N4 <sup>iii</sup>	121.07 (12)
O3—Zn1—O7	88.35 (10)	N4 <sup>iii</sup> —Zn3—N12 <sup>ii</sup>	106.99 (12)
O3—Zn1—O1	87.42 (10)	O10—Zn2—N9	113.12 (12)
O3—Zn1—N8 <sup>i</sup>	106.39 (12)	O10—Zn2—N5	104.43 (13)
N8 <sup>i</sup> —Zn1—O7	94.52 (11)	O8 <sup>iv</sup> —Zn2—O10	95.61 (11)
N8 <sup>i</sup> —Zn1—O1	97.04 (11)	O8 <sup>iv</sup> —Zn2—N9	119.77 (12)
O8 <sup>iv</sup> —Zn2—N5	110.91 (13)	N5—Zn2—N9	111.09 (13)

Symmetry codes **1**: (i) x-1, y, z; (ii) x-1, y, z-1; (iii) x+1, y, z; (iv) x+1, y, z+1.

Symmetry codes **2**: (i) x+1, 1/2-y, z+1/2; (ii) x+1, y, 1+z; (iii) 1-x, 1/2+y, 3/2-z; (iv) 1-x, 1-y, 1-z;  
(v) x-1, y, z-1; (vi) 1-x, y-1/2, 3/2-z; (vii) x-1, 1/2-y, z-1/2.

**Table S2.** Hydrogen bonding parameters of **1**.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 $\cdots$ O2	0.82	1.85	2.574 (3)	146
O7—H7A $\cdots$ O4	0.85	2.18	3.026 (3)	176
O7—H7B $\cdots$ O6 <sup>i</sup>	0.85	2.41	3.168 (4)	150

**Table S3.** Hydrogen bonding parameters of **2**.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O13—H13A $\cdots$ O6	0.85	1.97	2.807 (6)	167.3
O13—H13B $\cdots$ O14	0.85	1.97	2.816 (10)	170.3
O16—H16B $\cdots$ O2	0.85	2.16	2.999(6)	166.9
O14—H14A $\cdots$ O15	0.85	1.81	2.62(2)	158.5
O17—H17A $\cdots$ O5	0.85	2.08	2.923 (11)	173.5

**Table S4.** The CIE coordinates of the **1** and **1 @ M<sup>n+</sup>** in maximum emissions of **1** ( $\lambda_{\text{ex}}=323\text{nm}$ ). The CIE coordinates of the **2** and **2 @ M<sup>n+</sup>** in maximum emissions of **2** ( $\lambda_{\text{ex}}=311\text{nm}$ ).

Compound <b>1</b>	CIE coordinates	Compound <b>2</b>	CIE coordinates
<b>1 @ Ag<sup>+</sup></b>	(0.15, 0.06)	<b>2 @ Ag<sup>+</sup></b>	(0.16, 0.04)
<b>1 @ Al<sup>3+</sup></b>	(0.15, 0.05)	<b>2 @ Al<sup>3+</sup></b>	(0.15, 0.02)
<b>1 @ Ca<sup>2+</sup></b>	(0.15, 0.06)	<b>2 @ Ca<sup>2+</sup></b>	(0.16, 0.04)
<b>1 @ Cd<sup>2+</sup></b>	(0.15, 0.06)	<b>2 @ Cd<sup>2+</sup></b>	(0.16, 0.04)
<b>1 @ Co<sup>2+</sup></b>	(0.15, 0.06)	<b>2 @ Co<sup>2+</sup></b>	(0.16, 0.04)
<b>1 @ Cr<sup>3+</sup></b>	(0.15, 0.06)	<b>2 @ Cr<sup>3+</sup></b>	(0.16, 0.04)
<b>1 @ Cu<sup>2+</sup></b>	(0.15, 0.06)	<b>2 @ Cu<sup>2+</sup></b>	(0.16, 0.03)
<b>1 @ Fe<sup>3+</sup></b>	(0.15, 0.04)	<b>2 @ Fe<sup>3+</sup></b>	(0.16, 0.01)
<b>1 @ Hg<sup>2+</sup></b>	(0.15, 0.05)	<b>2 @ Hg<sup>2+</sup></b>	(0.13, 0.03)
<b>1 @ K<sup>+</sup></b>	(0.15, 0.06)	<b>2 @ K<sup>+</sup></b>	(0.16, 0.04)
<b>1 @ Li<sup>+</sup></b>	(0.15, 0.06)	<b>2 @ Li<sup>+</sup></b>	(0.16, 0.04)
<b>1 @ Mg<sup>2+</sup></b>	(0.15, 0.06)	<b>2 @ Mg<sup>2+</sup></b>	(0.16, 0.04)
<b>1 @ Mn<sup>2+</sup></b>	(0.15, 0.06)	<b>2 @ Mn<sup>2+</sup></b>	(0.16, 0.04)
<b>1 @ Ni<sup>2+</sup></b>	(0.15, 0.06)	<b>2 @ Ni<sup>2+</sup></b>	(0.16, 0.04)
<b>1 @ Pb<sup>2+</sup></b>	(0.15, 0.06)	<b>2 @ Pb<sup>2+</sup></b>	(0.16, 0.04)
<b>1 @ Zn<sup>2+</sup></b>	(0.15, 0.05)	<b>2 @ Zn<sup>2+</sup></b>	(0.16, 0.04)
blank	(0.15, 0.06)	blank	(0.16, 0.04)

**Table S5.** Comparison of detection capacities of **1** towards Fe<sup>3+</sup> ion with other materials.

Materials	K <sub>sv</sub> (M <sup>-1</sup> )	Detection limit	Ref.
{[Zn <sub>2</sub> (μ <sub>4</sub> -L)(μ <sub>3</sub> -bta(3H <sub>2</sub> O)]·H <sub>2</sub> O} <sub>n</sub>	1.06×10 <sup>4</sup>	1.1 mM	1
{[Zn(L) <sub>0.5</sub> (bimb)]·2H <sub>2</sub> O·0.5(CH <sub>3</sub> ) <sub>2</sub> NH} <sub>n</sub>	6.28 ×10 <sup>4</sup>	0.48 μM	2
{[Zn(L) <sub>0.5</sub> (btdpe)]·H <sub>2</sub> O} <sub>n</sub>	4.07 ×10 <sup>4</sup>	0.74 μM	2
[Zn <sub>3</sub> (DDB)(DPE)]·H <sub>2</sub> O	5.0 ×10 <sup>4</sup>	1.8 × 10 <sup>-7</sup> M	3
Tb(HL)(H <sub>2</sub> O) <sub>2</sub>	1.37 ×10 <sup>4</sup>	7.74 ×10 <sup>-4</sup> mM	4
[Zn(modbc) <sub>2</sub> ] <sub>n</sub> (Zn-CP)	7.20×10 <sup>3</sup>	0.57 mM	5
534-MOF-Tb	5.51×10 <sup>3</sup>	0.13 mM	6
[Zn(L) <sub>2</sub> ] <sub>n</sub>	1.34×10 <sup>4</sup>	2.24 μM	7
Eu <sup>3+</sup> @MIL-53-COOH (Al)	5.12 × 10 <sup>3</sup>	0.5 μM	8
Benzimidazole-based sensor	8.51 × 10 <sup>4</sup>	2 μM	9
BUT-14	2.17 × 10 <sup>3</sup>	3.8 μM	10
BUT-15	1.66 × 10 <sup>4</sup>	0.8μM	10
Eu <sub>2</sub> (MFDA) <sub>2</sub> (HCOO) <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	1.58 × 10 <sup>3</sup>	0.3 μM	11
<b>1</b>	4.16 × 10 <sup>4</sup>	1.66 μM	This work

**Table S6.** Comparison of detection capacities of **2** towards Hg<sup>2+</sup> ion with other materials.

Materials	K <sub>sv</sub> (M <sup>-1</sup> )	Detection limit	Ref.
[Cd(L)(NTA)] <sub>n</sub>	3.57×10 <sup>3</sup>	3.05 μM	12
[Ni(L)(NPTA)·H <sub>2</sub> O] <sub>n</sub>	7.43×10 <sup>3</sup>	2.29 μM	12
[Cd(2-NH <sub>2</sub> bdc)(tib)·4H <sub>2</sub> O·0.5DMA] <sub>n</sub>	-	4.2×10 <sup>-8</sup> M	13
{[Cd(BIPA)(tfbdc)(H <sub>2</sub> O)]·DMF} <sub>n</sub>	1.27 × 10 <sup>4</sup>	1.2 × 10 <sup>-7</sup> M	14
RuUiO-67	-	0.5 μM	15
[Zn <sub>2</sub> (bbmb) <sub>2</sub> (tdc) <sub>2</sub> ]·2H <sub>2</sub> O	4.81×10 <sup>5</sup>	0.19 μM	16
TbTATAB	-	4.4 nM	17
<b>2</b>	1.98 × 10 <sup>5</sup>	0.23 μM	This work

**Table S7.** The ICP result of polymer **2** with Hg<sup>2+</sup> for 6 hours.

Polymer <b>2</b>	Concentration /μM
Initial value / Hg <sup>2+</sup>	0.82
Immersion of Hg <sup>2+</sup> ions for 6 hours	0.46

**Table S8.** The proton conductivity of polymer **1** and **2** at 10 °C with different humidities.

Relative humidity (% RH)	Polymer <b>1</b> (S·cm <sup>-1</sup> )	Polymer <b>2</b> (S·cm <sup>-1</sup> )
45% RH	4.40×10 <sup>-7</sup>	4.68×10 <sup>-7</sup>
53% RH	5.51×10 <sup>-7</sup>	5.92×10 <sup>-7</sup>
62% RH	5.84×10 <sup>-7</sup>	6.67×10 <sup>-7</sup>
71% RH	9.51×10 <sup>-7</sup>	7.51×10 <sup>-7</sup>
83% RH	1.68×10 <sup>-6</sup>	8.01×10 <sup>-7</sup>
95% RH	7.87×10 <sup>-6</sup>	8.81×10 <sup>-7</sup>

**Table S9.** The proton conductivity of polymer **1** and **2** at 95% RH with different temperature.

Temperature	Polymer <b>1</b> (S·cm <sup>-1</sup> )	Polymer <b>2</b> (S·cm <sup>-1</sup> )
10°C	7.87×10 <sup>-6</sup>	8.81×10 <sup>-7</sup>
20°C	9.76×10 <sup>-6</sup>	1.49×10 <sup>-6</sup>
30°C	1.43×10 <sup>-5</sup>	2.21×10 <sup>-6</sup>
40°C	2.03×10 <sup>-5</sup>	3.69×10 <sup>-6</sup>
50°C	2.91×10 <sup>-5</sup>	4.79×10 <sup>-6</sup>
60°C	3.45×10 <sup>-5</sup>	6.26×10 <sup>-6</sup>

**Table S10.** Summarized proton conductivities of some MOFs at high humidity (>80% RH)

Materials	Proton conductivity (S·cm <sup>-1</sup> )	RH and Temperature (°C)	Ref.
MIL-53(Fe)(COOH) <sub>2</sub>	1.5×10 <sup>-3</sup>	95% and 80	18
[Cd(L-tart)-(bpy)(H <sub>2</sub> O)] <sub>n</sub> ·9n(H <sub>2</sub> O)	1.3×10 <sup>-6</sup>	95% and 85	19
[Cd(D-tart)-(bpy)(H <sub>2</sub> O)] <sub>n</sub> ·9n(H <sub>2</sub> O)	1.3×10 <sup>-6</sup>	95% and 85	19
[Cd(DL-tart)-(bpy)(H <sub>2</sub> O)] <sub>n</sub> ·6n(H <sub>2</sub> O)	4.5×10 <sup>-7</sup>	95% and 85	19
{[Gd(L)(Ox)(H <sub>2</sub> O)] <sub>n</sub> ·3H <sub>2</sub> O}	4.7×10 <sup>-4</sup>	95% and 80	20
Tb-DSOA	4.0×10 <sup>-4</sup>	98% and 53	21
β-PCMOF2	1.8×10 <sup>-6</sup>	85% and 50	22
PCMOF2	2.4×10 <sup>-5</sup>	85% and 50	22
PCMOF-3	3.5×10 <sup>-5</sup>	98% and 25	23
Sr-SBBA	4.4×10 <sup>-5</sup>	98% and 25	24
[La <sub>2</sub> (ox) <sub>3</sub> (H <sub>2</sub> O) <sub>6</sub> ] 4H <sub>2</sub> O	3.35×10 <sup>-7</sup>	100% and 95	25
[Zn <sub>2</sub> (HCOO)(trz) <sub>3</sub> ] <sub>n</sub>	7.95×10 <sup>-7</sup>	98% and 50	26
<b>1</b>	3.45×10 <sup>-5</sup>	95% and 60	This work
<b>2</b>	6.26×10 <sup>-6</sup>	95% and 60	This work

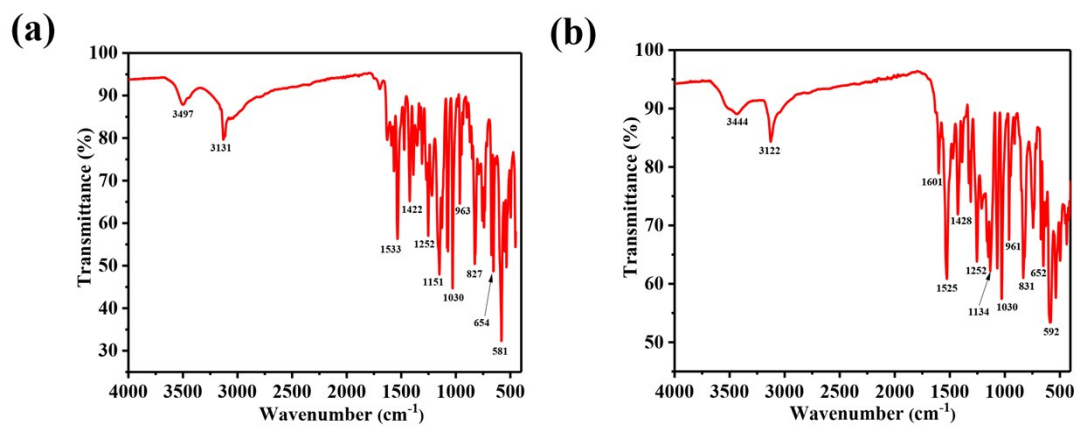


Fig. S1 (a) The IR spectra of 1. (b) The IR spectra of 2.

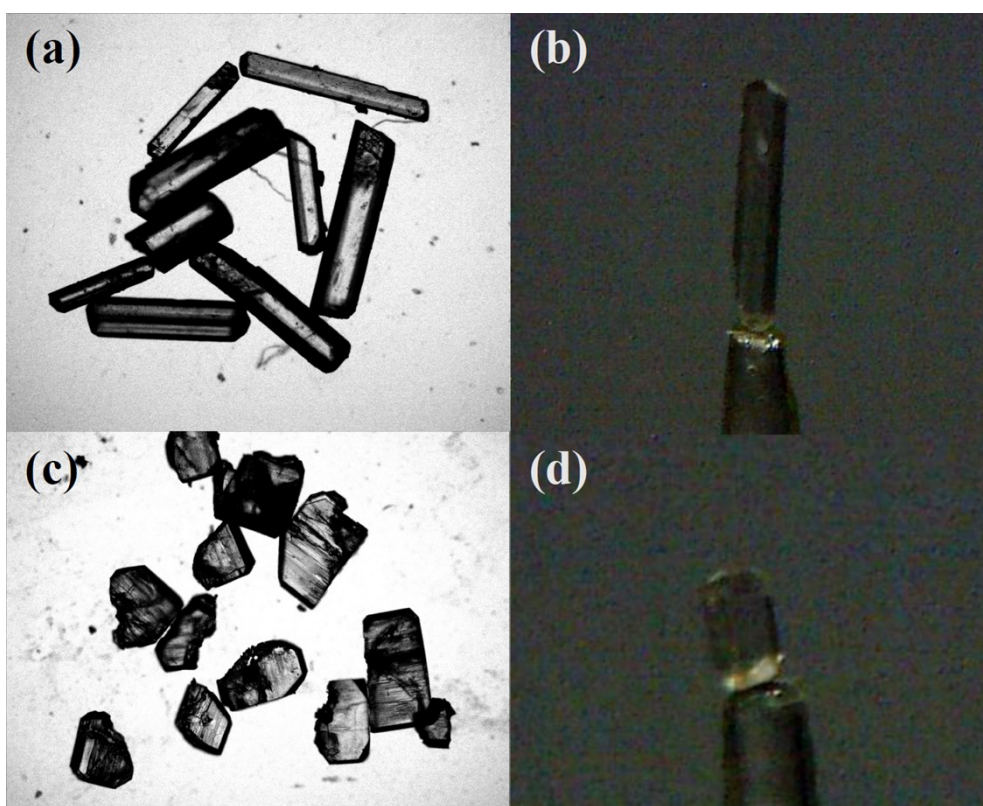
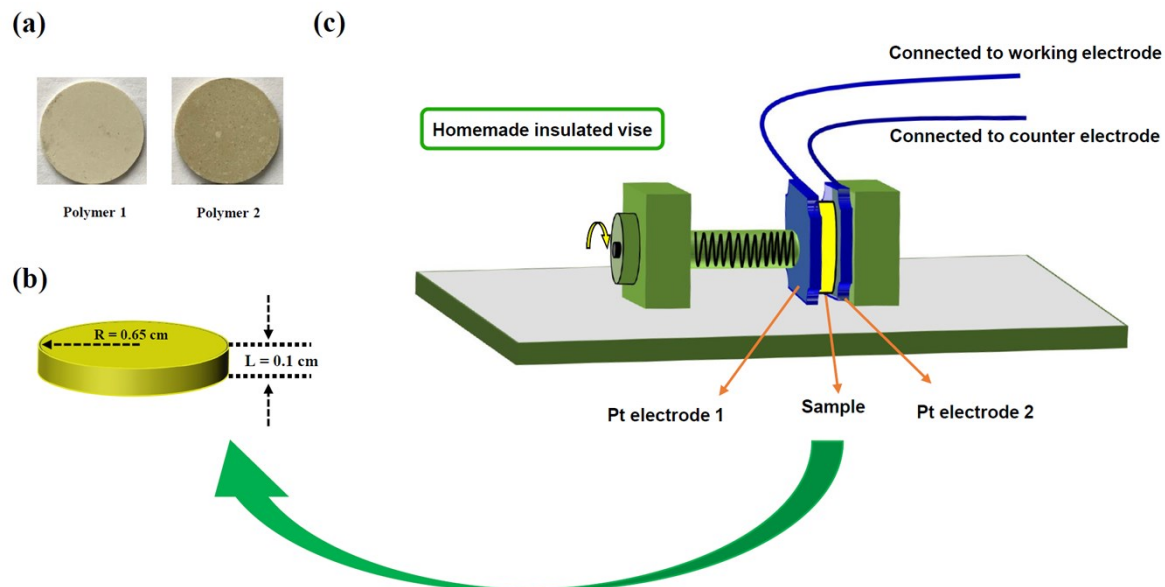
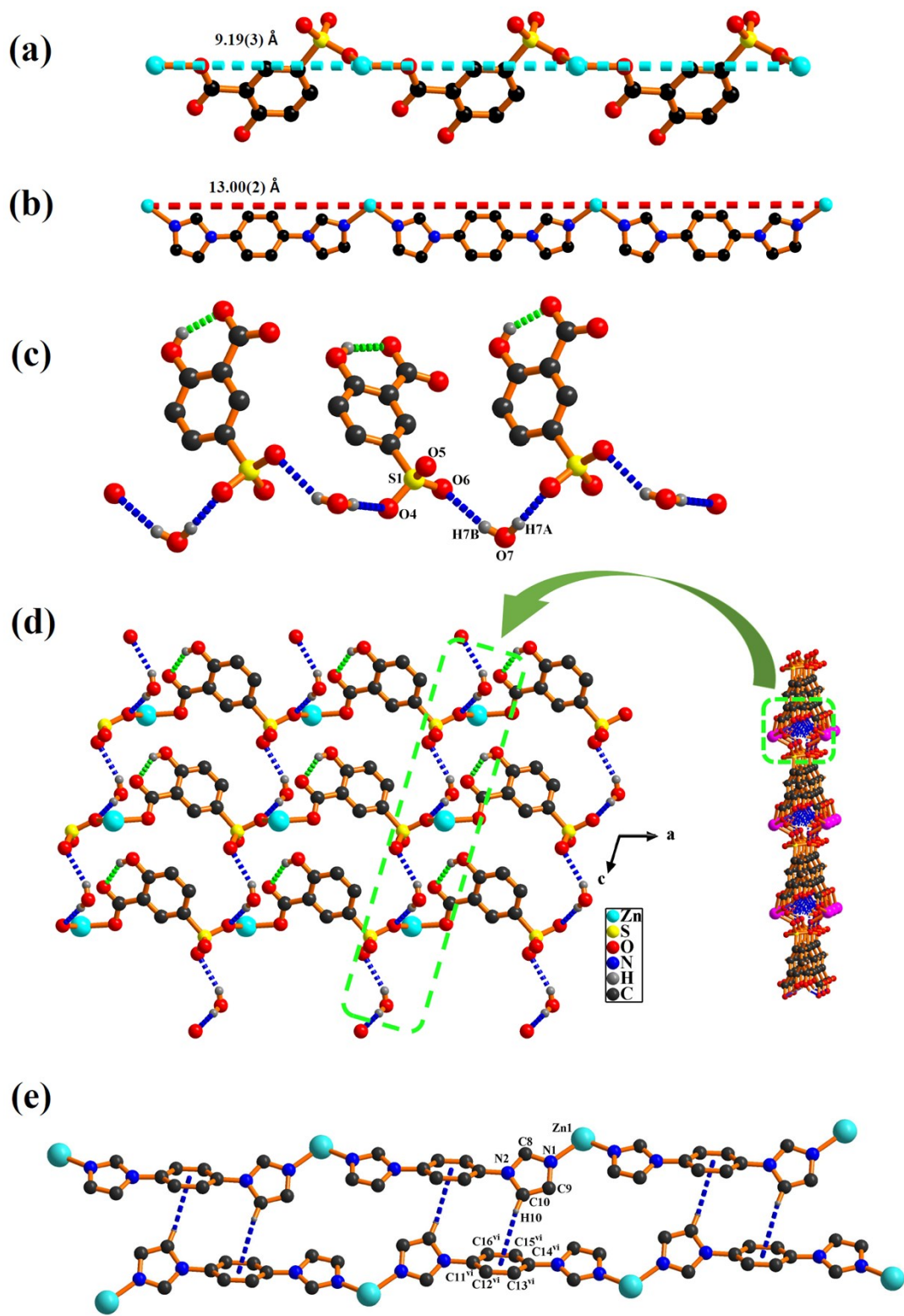


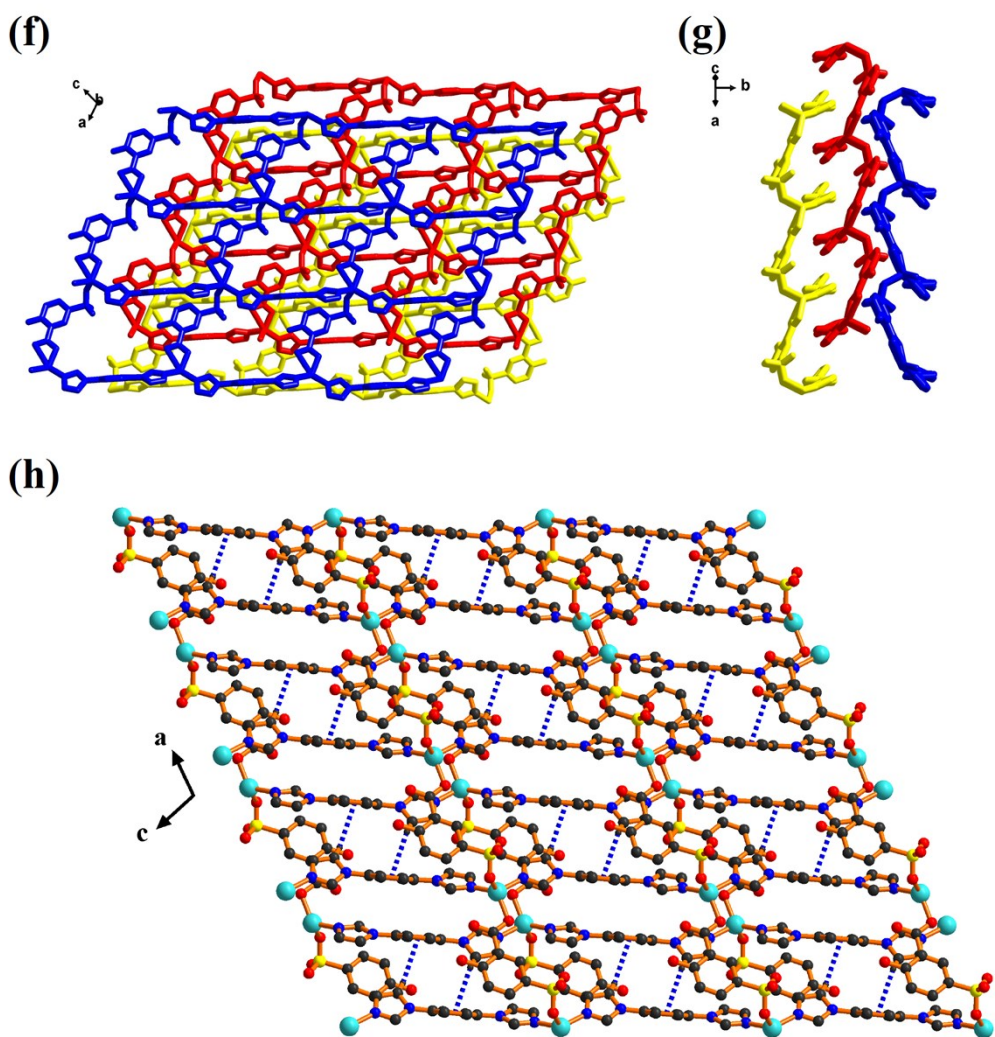
Fig. S2 Sample crystal photographs of polymer 1 (a) and polymer 2 (c). Single-crystal photographs of polymer 1 (b) and polymer 2 (d).



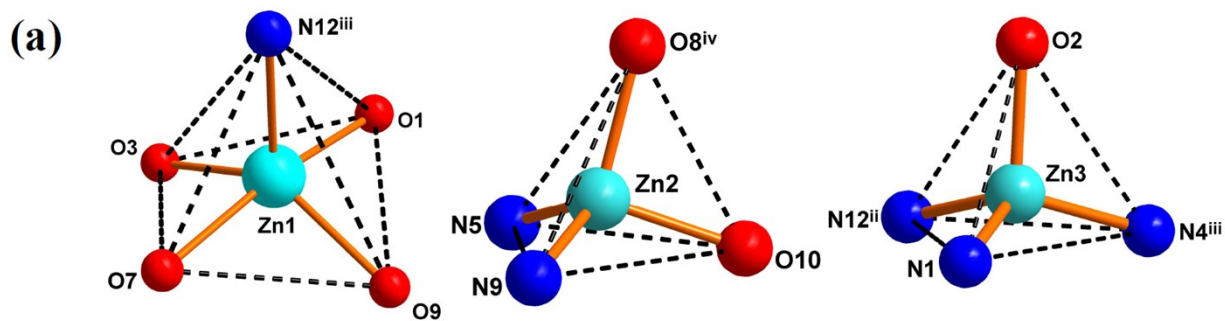
**Fig. S3** (a) Photographs of wafer press plates for polymers 1 and 2; (b) schematic diagram of wafer samples used for proton conductivity; (c) the home-made device for a proton conductivity test.

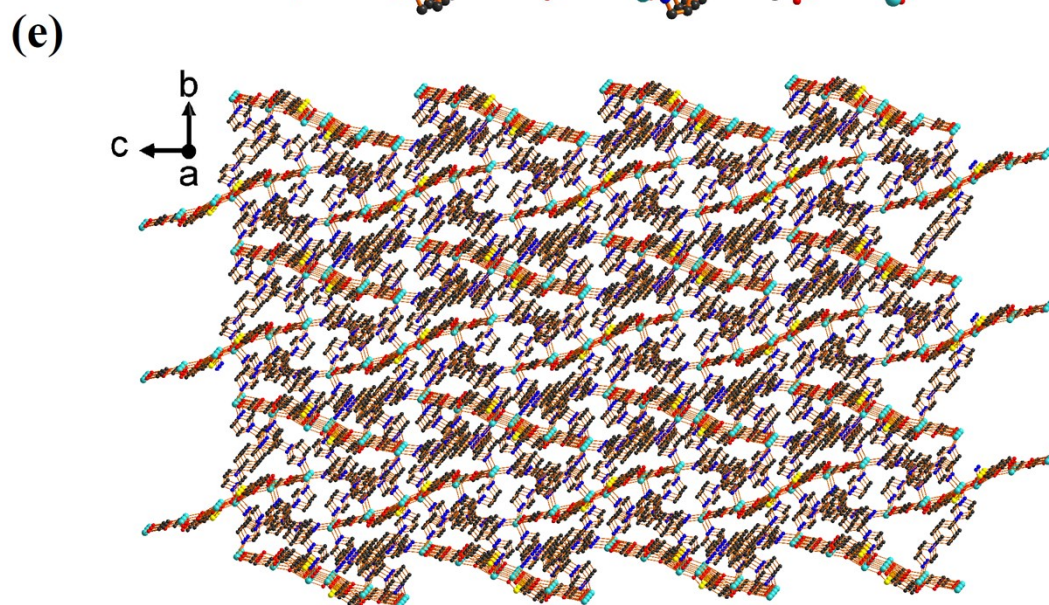
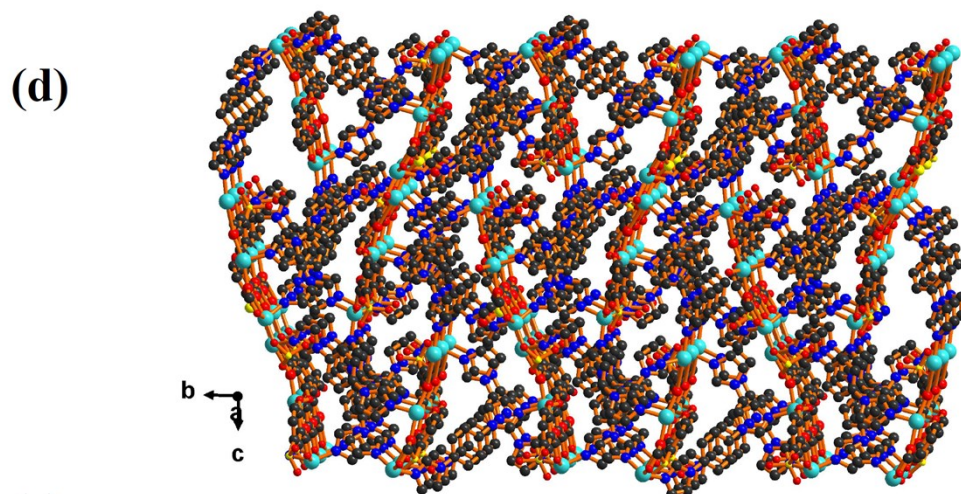
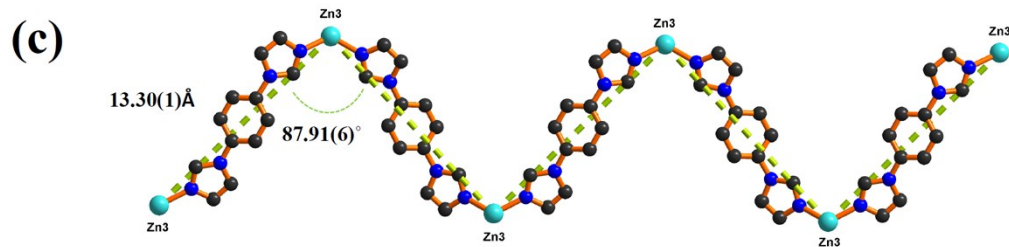
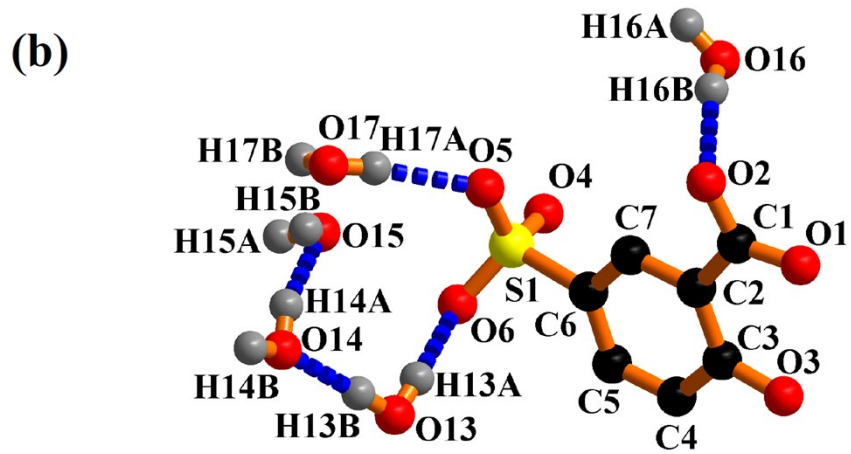




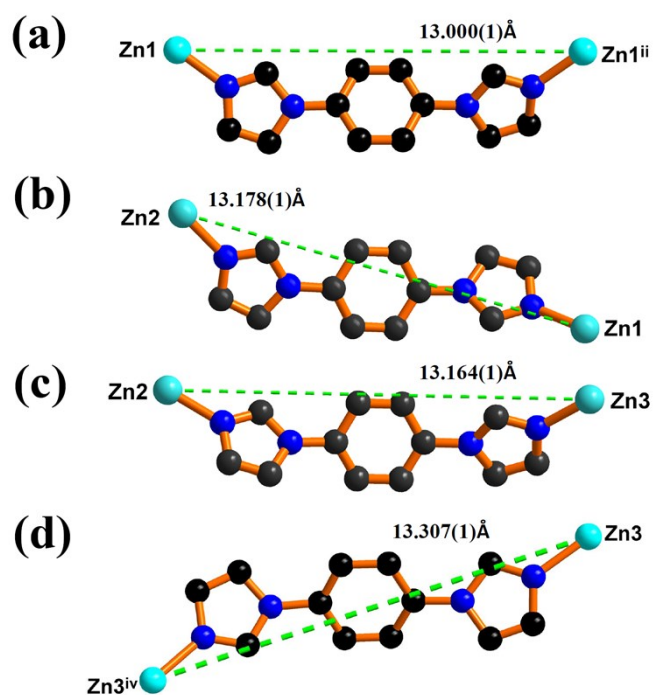


**Fig. S4** (a) The 1D  $[\text{Zn}(\text{H}_3\text{ssa})_n]$  chain in polymer **1**; (b) the 1D  $[\text{Zn}(1,4\text{-bib})_n]$  chain in polymer **1**; (c) the hydrogen-bonded passageway of polymer **1**; (d) the 2D H-bonded framework; (e) the C-H... $\pi$  interactions of polymer **1**; (f) the 3D structure framework of polymer **1** viewed in the direction *b*; (g) the 3D structure framework of polymer **1** viewed in the vertical *b* direction; (h) the 2D C-H... $\pi$  interactions of polymer **1**.

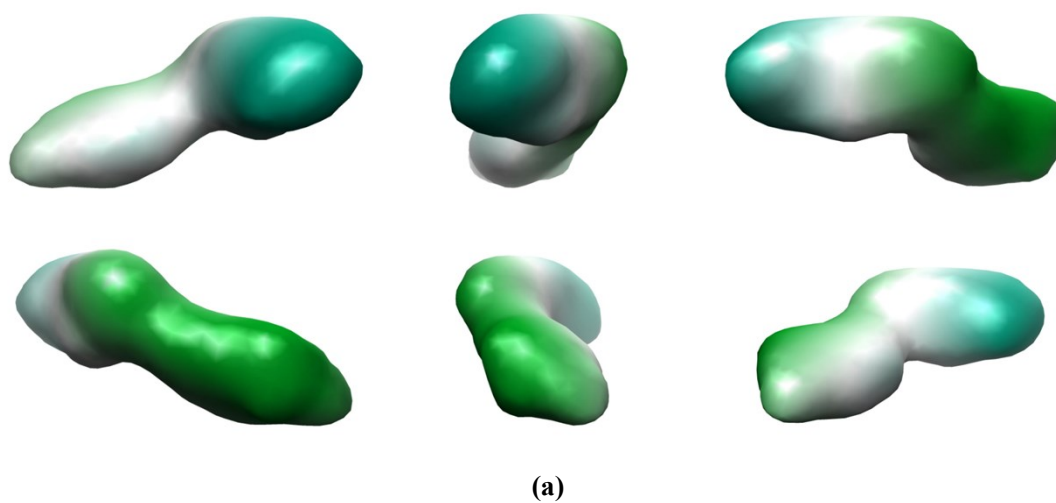


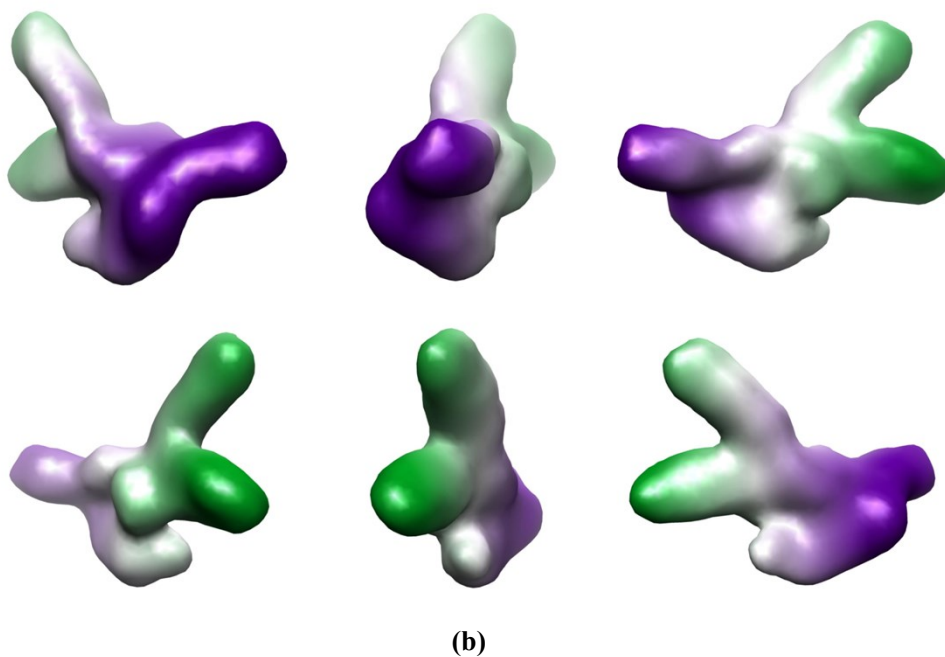


**Fig. S5** (a) Polyhedral view of polymer **2**; (b) The intermolecular O–H···O hydrogen bonds in polymer **2**. (c) the 1D  $[\text{Zn}(1,4\text{-bib})_n]$  chain in polymer **2**; (d) the first simplified method of polymer **2**, and the 3D structural framework corresponding to the topology; (e) the second simplified method of polymer **2**, and the 3D structural framework corresponding to the topology.

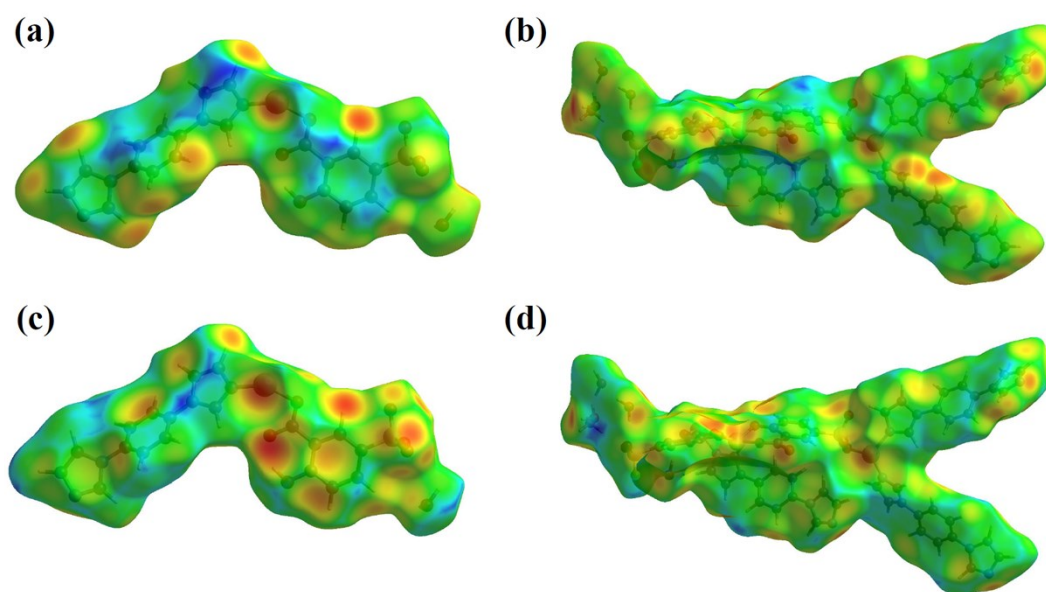


**Fig. S6** (a) The 1,4-bib ligand connector of the polymer **1**; (b-d) the 1,4-bib ligand connector of the polymer **2**.

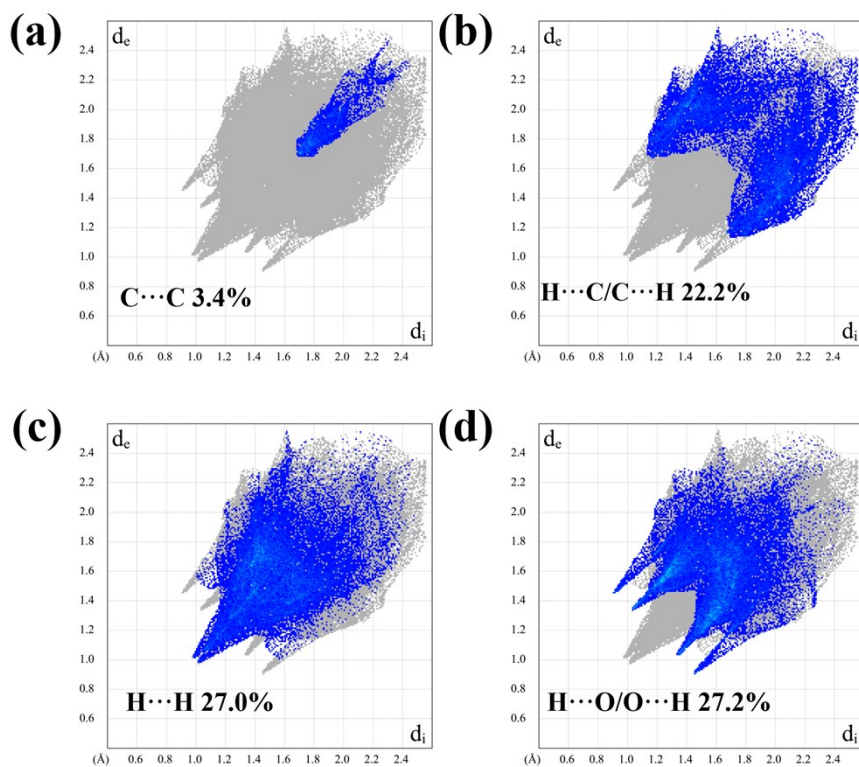




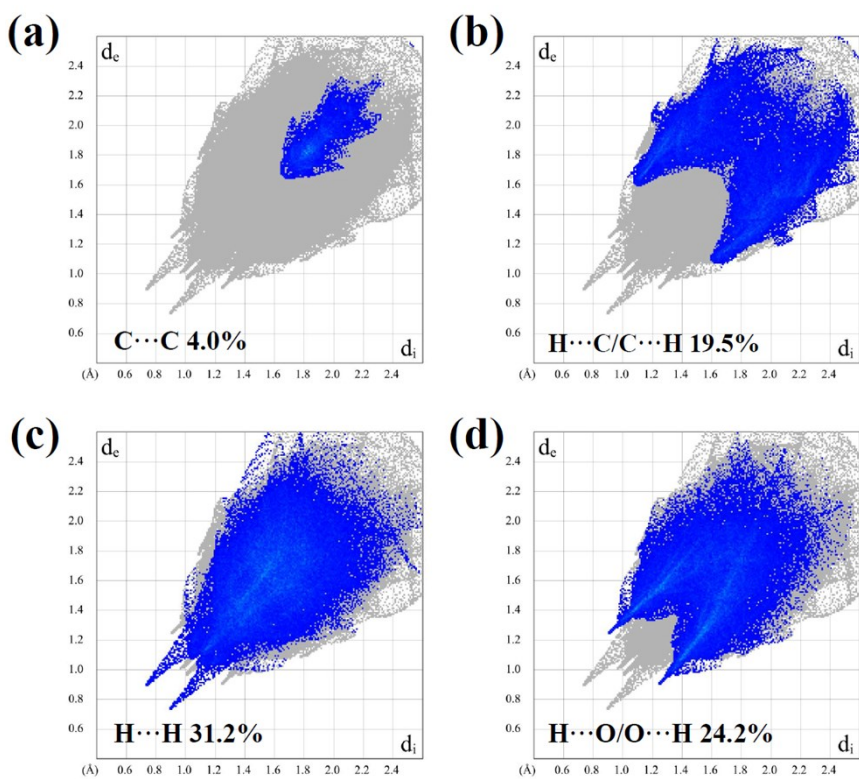
**Fig. S7** The surface of **1** (a) and **2** (b) calculated via 3V Volume Assessor program by rolling a virtual probe (0.8 Å) on the surface viewed along six different orientations.



**Fig. S8** Hirshfeld surface of polymer **1** with  $d_i$  (a),  $d_e$  (c) mapped in colour; the Hirshfeld surface of polymer **2** with  $d_i$  (b),  $d_e$  (d) mapped in colour; in all cases, red represents the closest contacts, and blue the most distant contacts.



**Fig. S9** Fingerprint plot of polymer **1**: resolved into  $C \cdots C$  (a),  $H \cdots C / C \cdots H$  (b),  $H \cdots H$  (c), and  $H \cdots O / O \cdots H$  (d) contacts showing the percentages of contacts contributed to the total Hirshfeld surface area of the molecule.



**Fig. S10** Fingerprint plot of polymer **2**: resolved into  $C \cdots C$  (a),  $H \cdots C / C \cdots H$  (b),  $H \cdots H$  (c), and  $H \cdots O / O \cdots H$  (d) contacts showing the percentages of contacts contributed to the total Hirshfeld surface area of the molecule.

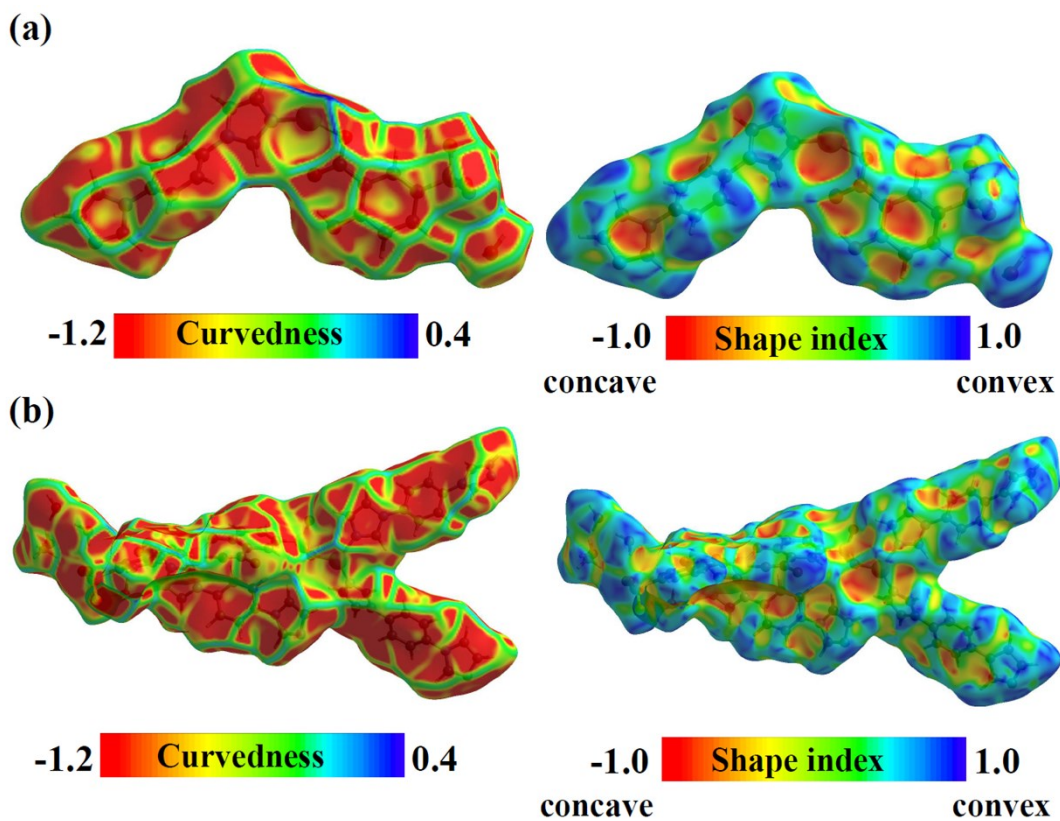


Fig. S11 (a) Hirshfeld surface of polymer 1 with curvedness and shape index mapping; (b) the Hirshfeld surface of polymer 2 with curvedness and shape index mapping.

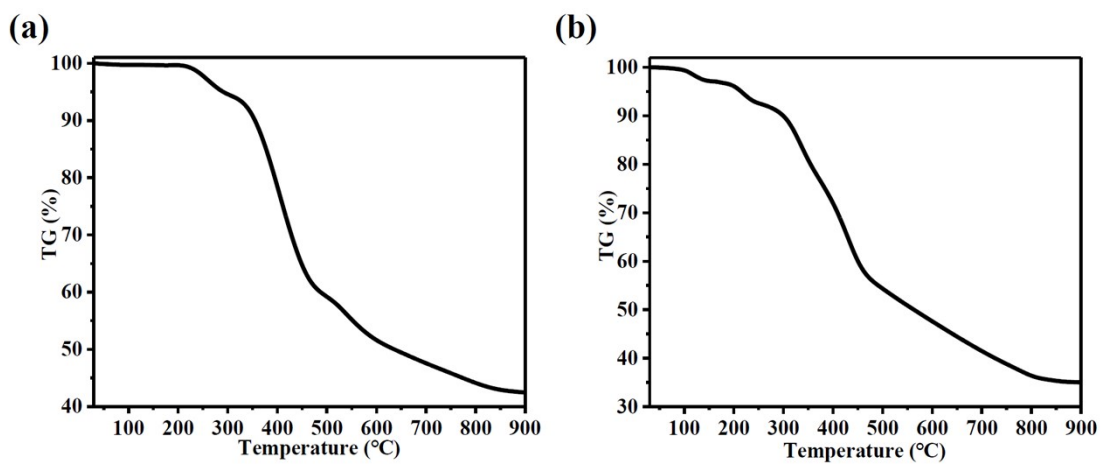


Fig. S12 The TG curves for 1 (a) and 2 (b).

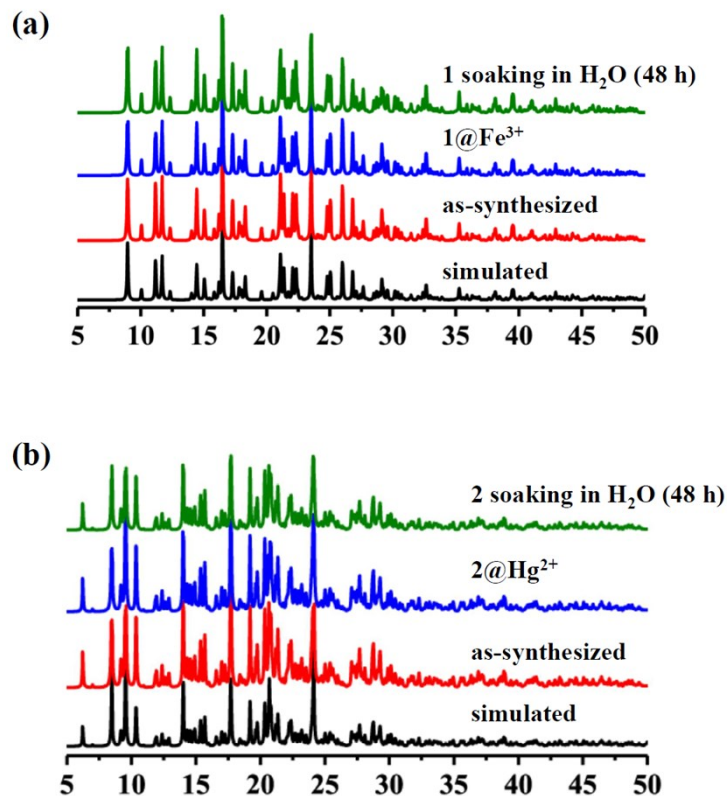


Fig. S13 The PXRD patterns of polymers 1 and 2.

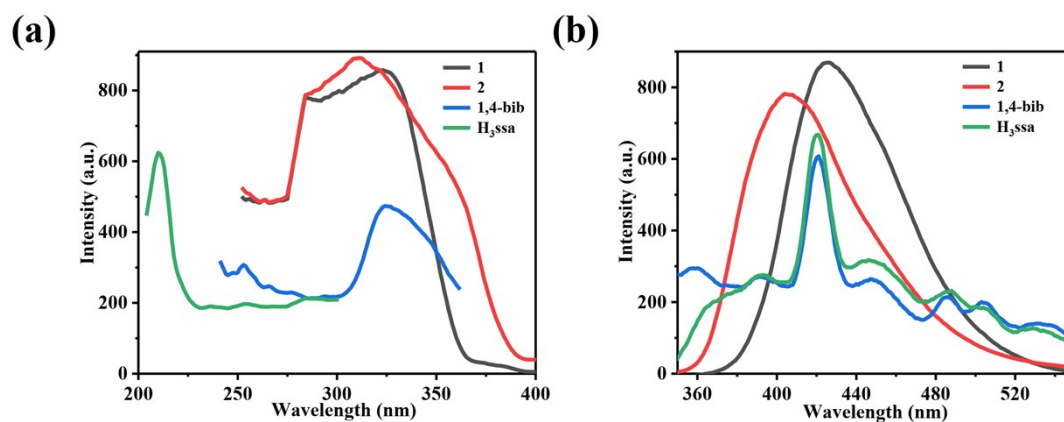
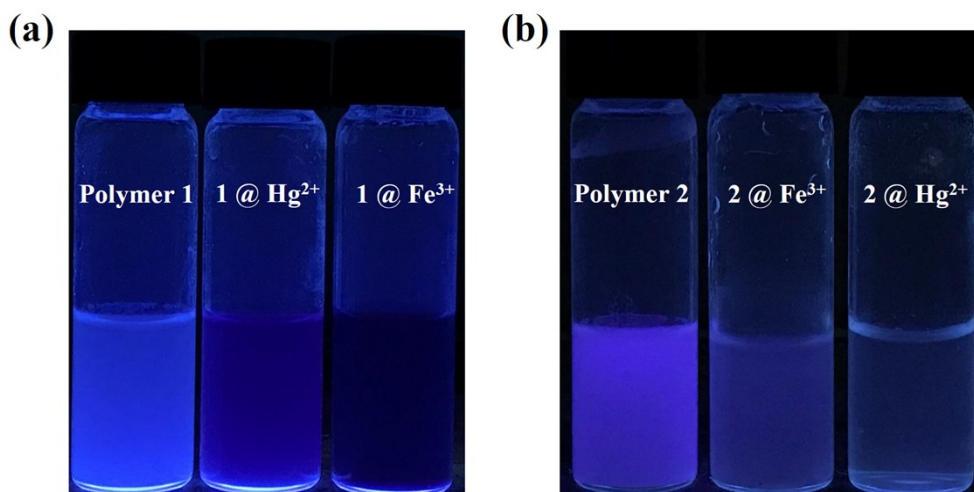
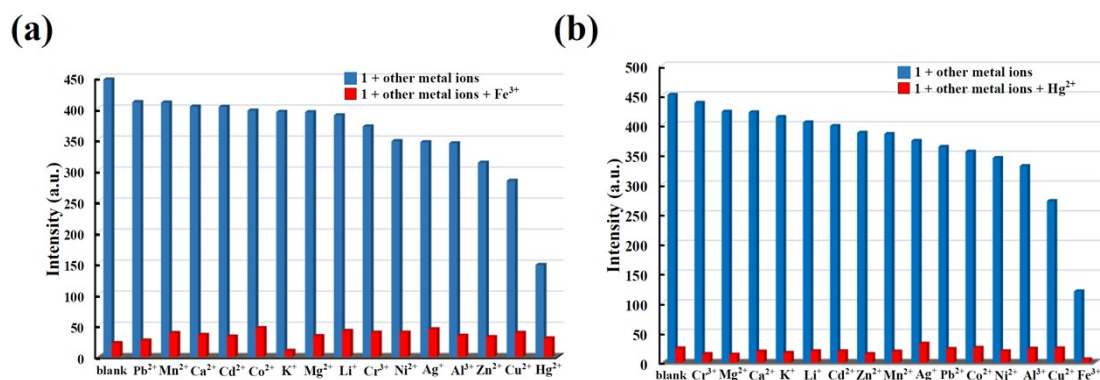


Fig. S14 (a) The solid-state excitation spectra of H<sub>3</sub>ssa ( $\lambda_{\text{ex}} = 210$  nm), 1,4-bib ( $\lambda_{\text{ex}} = 324$  nm), **1** ( $\lambda_{\text{ex}} = 323$  nm), and **2** ( $\lambda_{\text{ex}} = 311$  nm) at room temperature, (b) the solid-state emission spectra of H<sub>3</sub>ssa ( $\lambda_{\text{em}} = 420$  nm), 1,4-bib ( $\lambda_{\text{em}} = 420$  nm), **1** ( $\lambda_{\text{em}} = 425$  nm), and **2** ( $\lambda_{\text{em}} = 405$  nm) at room temperature.

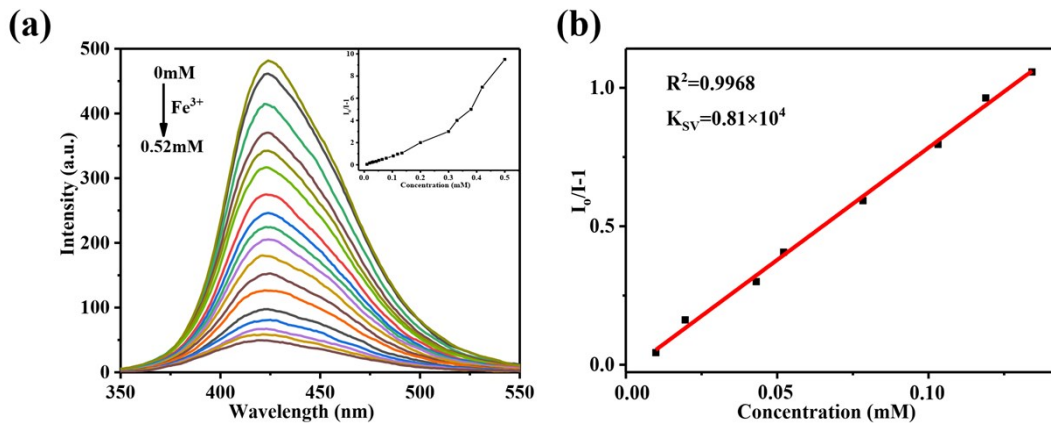




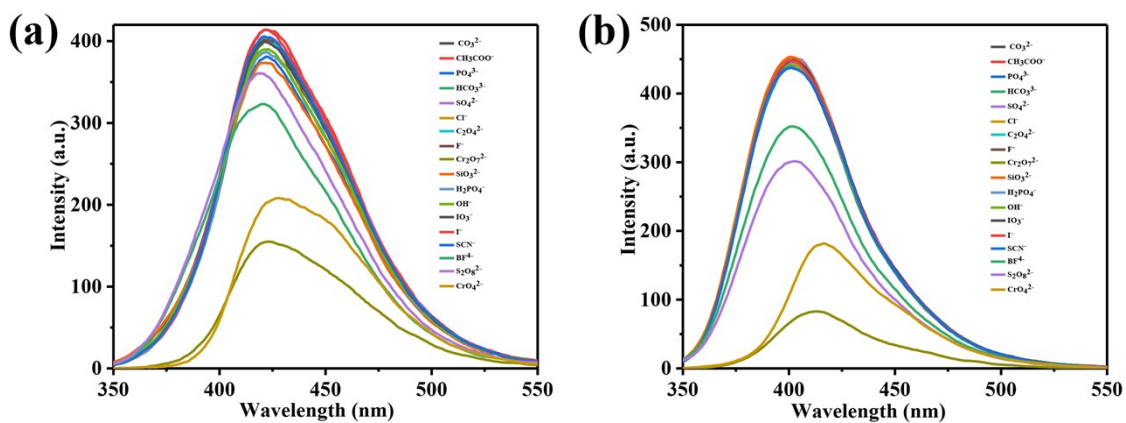
**Fig. S15** (a) The photograph of polymer 1, 1@Hg<sup>2+</sup>, and 1@Fe<sup>3+</sup> samples in water under UV light of 300 nm; (b) the photograph of polymer 2, 2@Fe<sup>3+</sup>, and 2@Hg<sup>2+</sup> samples in water under UV light of 365 nm.



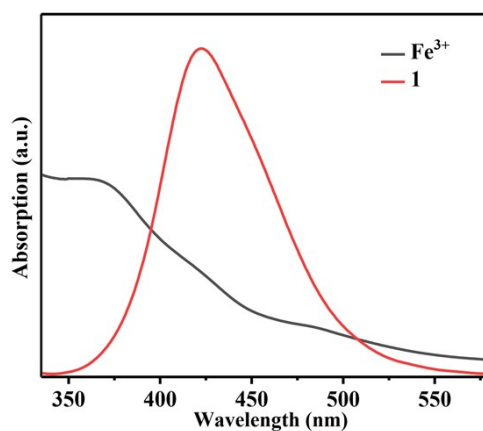
**Fig. S16** (a) The relative emission intensity of polymer 1 before and after addition Fe<sup>3+</sup> (1.5ml, 10<sup>-3</sup> M) and other metal ions (1.5ml, 10<sup>-3</sup> M); (b) the relative emission intensity of polymer 2 before and after addition Hg<sup>2+</sup> (1.5ml, 10<sup>-3</sup> M) and other metal ions (1.5ml, 10<sup>-3</sup> M).



**Fig. S17** (a) Fluorescent spectra of polymer **1** in simulated biological systems in the presence of different concentrations of  $\text{Fe}^{3+}$  at  $37^\circ\text{C}$ ; (b) emission quenching linearity relationship at low concentrations of  $\text{Fe}^{3+}$  ion for polymer **1** in simulated biological systems.



**Fig. S18** The photoluminescence spectra for polymer **1** (a) and **2** (b) in aqueous solution with various anions.



**Fig. S19** UV-Vis absorption spectra of  $\text{Fe}^{3+}$  in aqueous solution.

the emission spectrum of polymer **1** dispersed in water upon excitation of 323 nm.

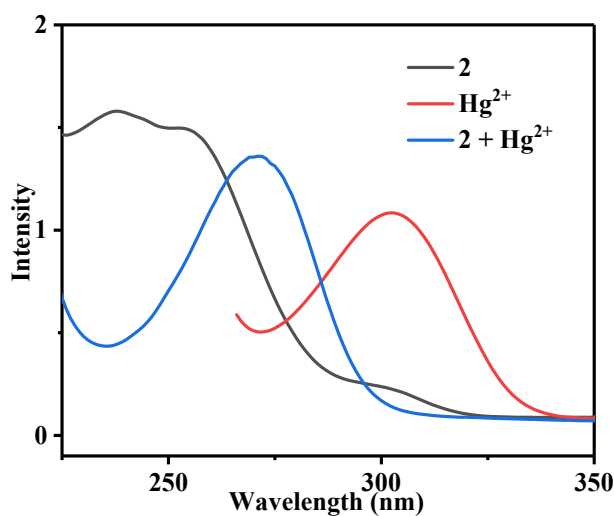


Fig. S20 UV-vis spectra of polymer **2** before and after addition of  $\text{Hg}^{2+}$  ion.

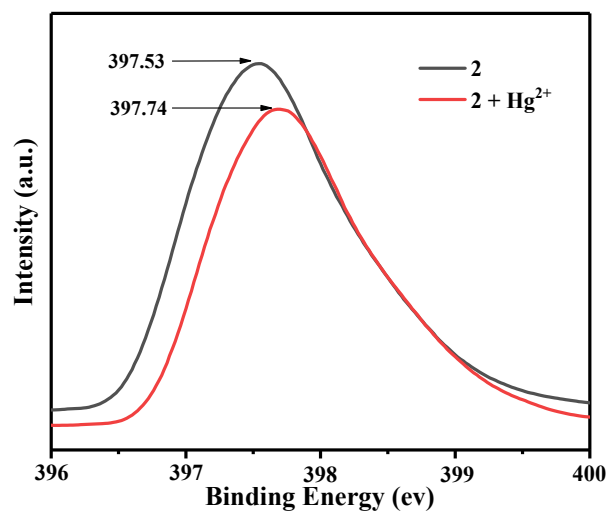


Fig. S21 N 1s XPS spectra of polymer **2** before and after immersed in  $\text{Hg}^{2+}$  ion.

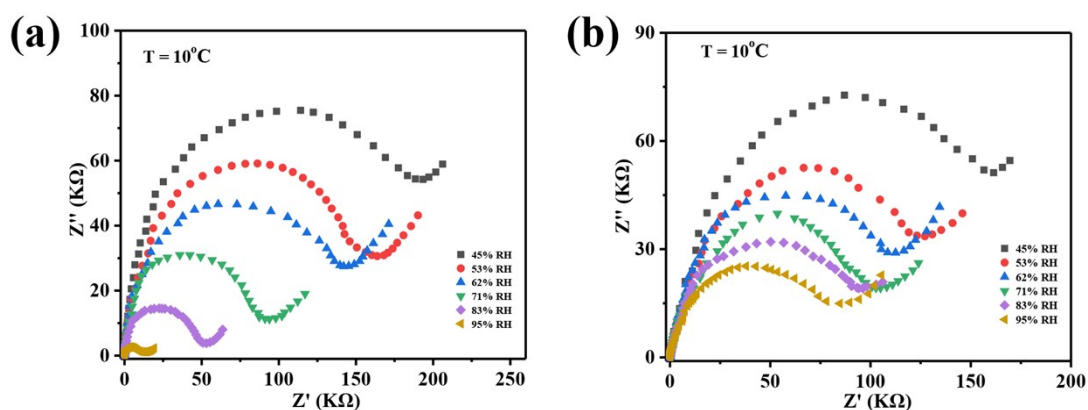
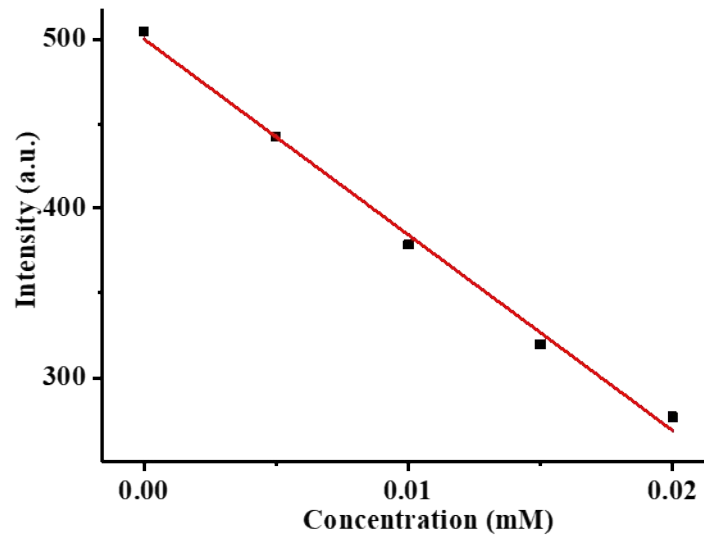


Fig. S22 (a) The Nyquist plots for polymer **1** at  $10^\circ\text{C}$  at different relative humidity; (b) the Nyquist plots for polymer **2** at  $10^\circ\text{C}$  at different relative humidity.

**Detection limit calculation process:**



(a) Corresponding Stern-Volmer plot for polymer **1** when  $\text{Fe}^{3+}$  ions are added

Linear Equation:  $Y = -11566.87X + 506.7$

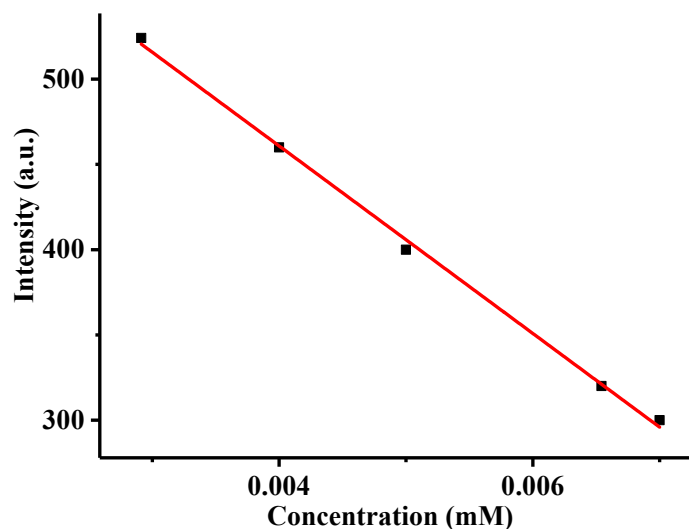
$$k = 1.1567 \times 10^7 \text{ M}^{-1}$$

$$I_a = \frac{498.3 + 505.1 + 492.9 + 496.2 + 508.7 + 500.1 + 513.1 + 502.7 + 507.9 + 497.2}{10} = 502.22$$

$$S = \sqrt{\frac{\sum (I_0 - I_a)^2}{N - 1}} = 6.41 \quad (N=10)$$

$$\text{LOD} = \frac{3 \times S}{k} = \frac{3 \times 6.41}{1.1567 \times 10^7} = 1.66 \mu\text{M}$$

$k$  is the slope of the calibration curve,  $I_0$  is the measured luminescence intensity of polymer **1** in deionized water,  $I_a$  is the average of 10 blank samples tested.  $S$  is the standard deviation of the blank group, LOD is the detection limit.



(b) Corresponding Stern-Volmer plot for polymer **2** when  $\text{Hg}^{2+}$  ions are added

Linear Equation:  $Y = -54978.79X + 578.7$

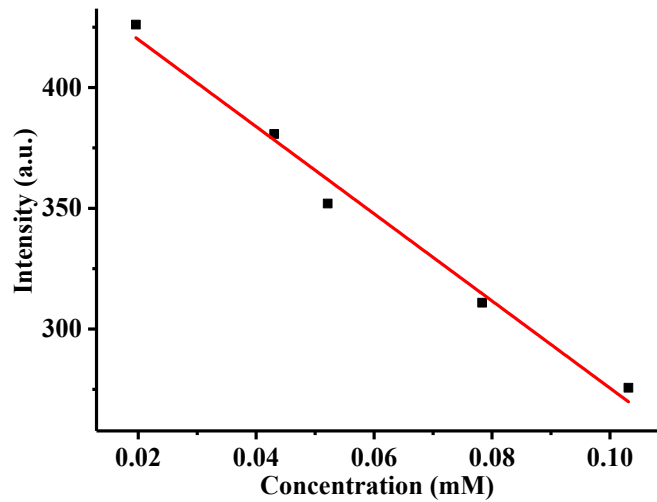
$$k=5.4979 \times 10^7 \text{ M}^{-1}$$

$$I_a = \frac{581.2 + 579.8 + 575.4 + 580.1 + 578.2 + 577.4 + 576.2 + 578.1 + 566.7 + 580.2}{10} = 577.33$$

$$S = \sqrt{\frac{\sum (I_0 - I_a)^2}{N - 1}} = 4.17 \quad (N=10)$$

$$\text{LOD} = \frac{3 \times S}{k} = \frac{3 \times 4.17}{5.4979 \times 10^7} = 0.23 \text{ } \mu\text{M}$$

$k$  is the slope of the calibration curve,  $I_0$  is the measured luminescence intensity of polymer **2** in deionized water,  $I_a$  is the average of 10 blank samples tested.  $S$  is the standard deviation of the blank group, LOD is the detection limit.



(c) Corresponding Stern-Volmer plot for polymer **1** when  $\text{Fe}^{3+}$  ions are added in biological systems

$$\text{Linear Equation: } Y = -1804.69X + 495.2$$

$$k = 1.80469 \times 10^6 \text{ M}^{-1}$$

$$I_a = \frac{499.7 + 490.2 + 500.1 + 495.4 + 492.3 + 497.4 + 494.5 + 498.1 + 499.4 + 489.7}{10} = 495.68$$

$$S = \sqrt{\frac{\sum (I_0 - I_a)^2}{N - 1}} = 3.90 \quad (N=10)$$

$$\text{LOD} = \frac{3 \times S}{k} = \frac{3 \times 3.90}{1.80469 \times 10^6} = 6.48 \text{ } \mu\text{M}$$

$k$  is the slope of the calibration curve,  $I_0$  is the measured luminescence intensity of polymer **1** in HEPES,  $I_a$  is the average of 10 blank samples tested.  $S$  is the standard deviation of the blank group,

LOD is the detection limit.

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