Supporting Information

A Europium(III) Based Metal-Organic Framework: Bifunctional Properties Related to Sensing and Electronic Conductivity

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Impedance test

The powders of I_2-incorporated **EuL** were prepared by grinding the sample into a homogeneous powder with a mortar and pestle. The powders were then added to a standard 8 mm die, sandwiched between two stainless steel electrodes and pressed at 5,000 kg for 5 min. the pellet was 8 mm in diameter and 1.2 mm in thickness. Conductivity was calculated using the following equation:

$$\sigma = \frac{l}{RsS}$$

where ***l*** and ***S*** are the thickness (cm) and cross-sectional area (cm^2) of the pellet respectively, and ***R*s**, which was extracted directly from the impedance plots, is the bulk resistance of the sample (**σ**).

There are four principle elements that contribute to the impedance behaviour of a material. Among the principle elements, three are resistors (R), capacitors (C) and inductors (L). The constant phase element (CPE) represented by Q, is the fourth element that can contribute to the overall impedance of a system. The elements R, C, L and Q can be used to design an equivalent circuit model to represent the impedance behaviour of a Nyquist plot. For the Nyquist plots of I_2-incorporated **EuL**, it is difficult to give only one equivalent circuit for the samples under different temperatures, because the deviation of the values for R, C, L and Q would be very large in that case. Thus, maybe different equivalent circuits were employed to calculate conductivity values for the samples under different temperatures. For example, the Nyquist plots for I_2-incorporated **EuL** at 25 °C have used the following equivalent circuit which has been used by Ma's group.[1] For different Nyquist plots, the fundamental rule of the equivalent circuits is that the deviation of the values for R, C, L and Q must be less than 10% on the condition of without deviating the basic principles.

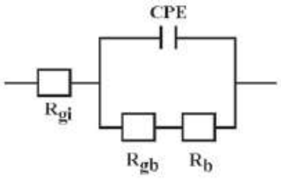

Figure S1. a) Polyhedral representation of **EuL**; b) a distorted monocapped square antiprism which is formed by Eu1 in **EuL**; c) a distorted square antiprism which is formed by Eu2 (Eu3 or Eu4) in **EuL**.

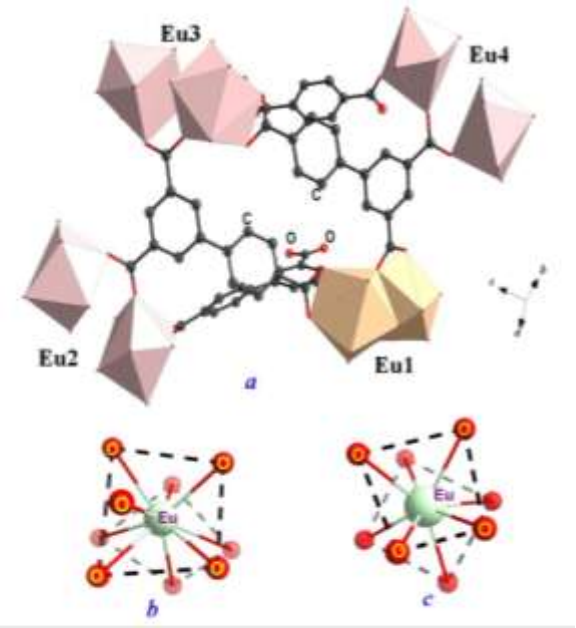

Figure S2. The representation of the coordination environments for Eu atoms in **EuL**: a) Eu1; b) Eu2; c) Eu3; d) Eu4.

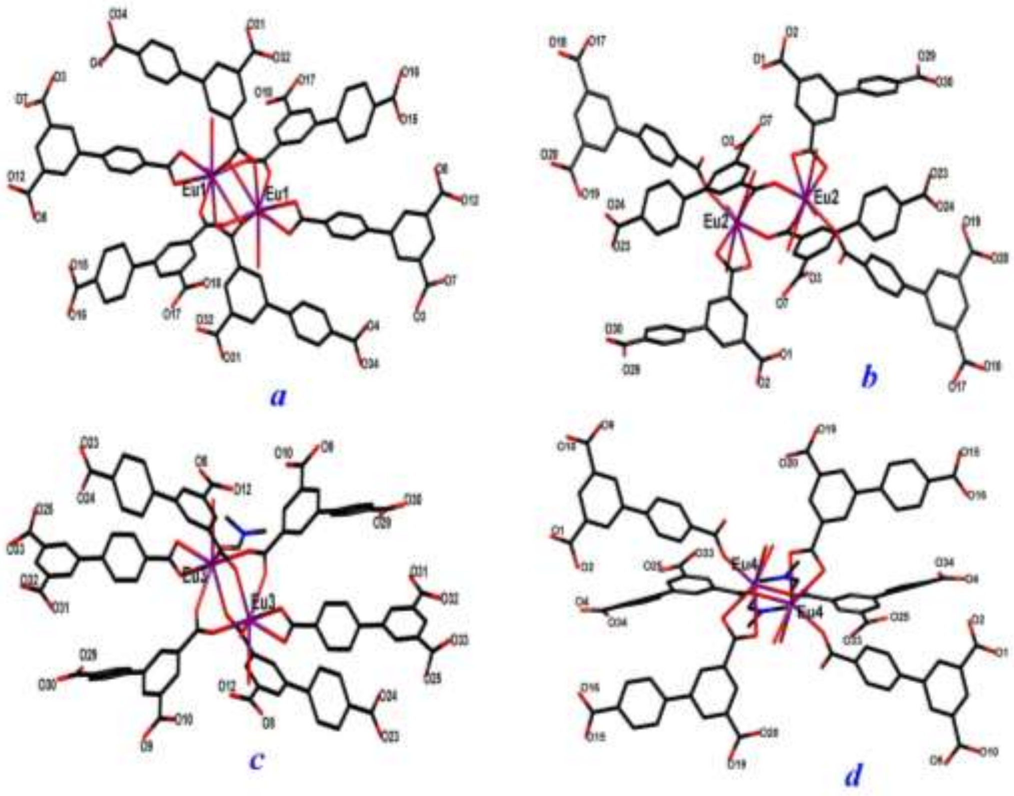

Figure S3. The TG curve for solid I_2.

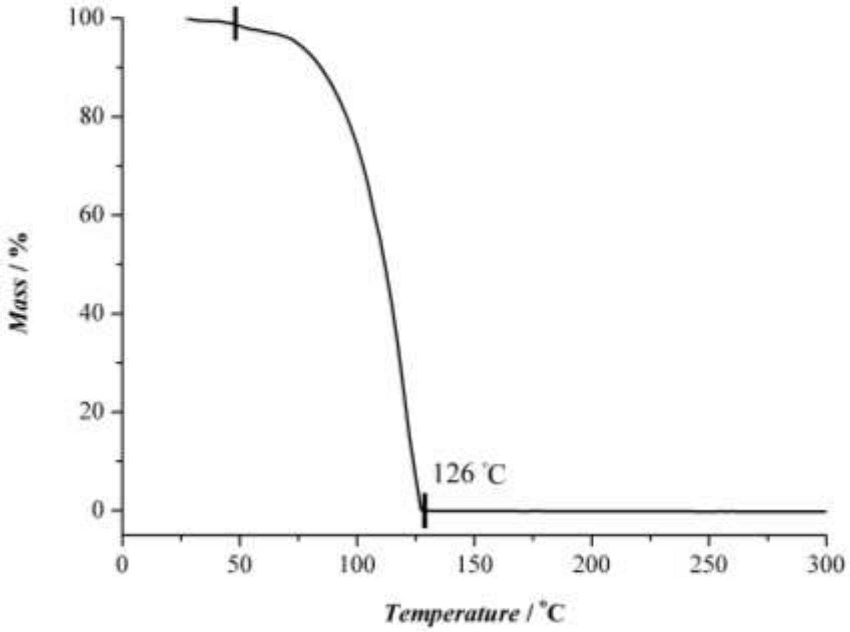

Figure S4. N_2 adsorption isotherm of **EuL** at 77 K.

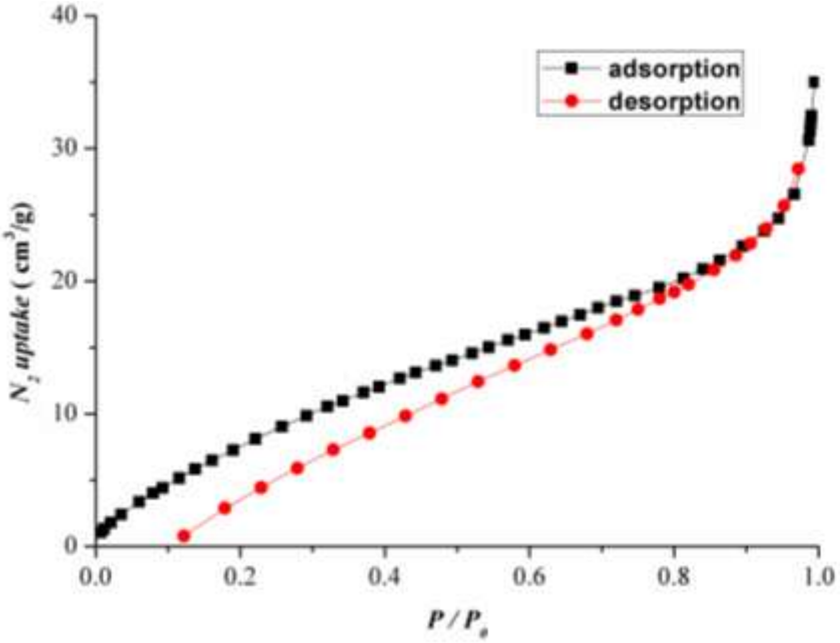

Figure S5. The luminescence spectrum of **EuL** in DMF solution at different Cu^{2+} concentrations.

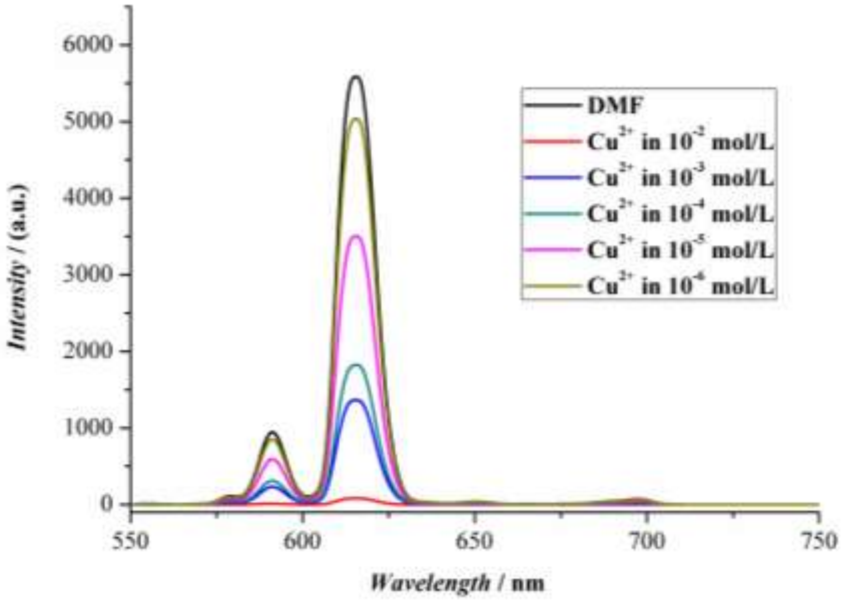

Figure S6. Powder XRD patterns of representative samples. As shown in the figure, the outgassed **EuL** remains highly crystallized and retains the main framework features of **EuL** but with lost of several peaks. This is probably due to the distortion or shrinking of the crystal lattice to some degree in response to heating and removal of guest molecules, which is commonly observed in a lot of MOF structures. Comparing with the outgassed **EuL**, I_2-incorporated **EuL** also remains highly crystallized and retains the main framework features of **EuL**, but the differences are that a few new peaks have arisen. This is probably due to that the distortion or shrinking of the crystal lattice was re-plumped up because of the immersion of I_2. Moreover, the similar process also happened to the samples of Cu^{2+}-incorporated **EuL** and acetone-incorporated **EuL**.

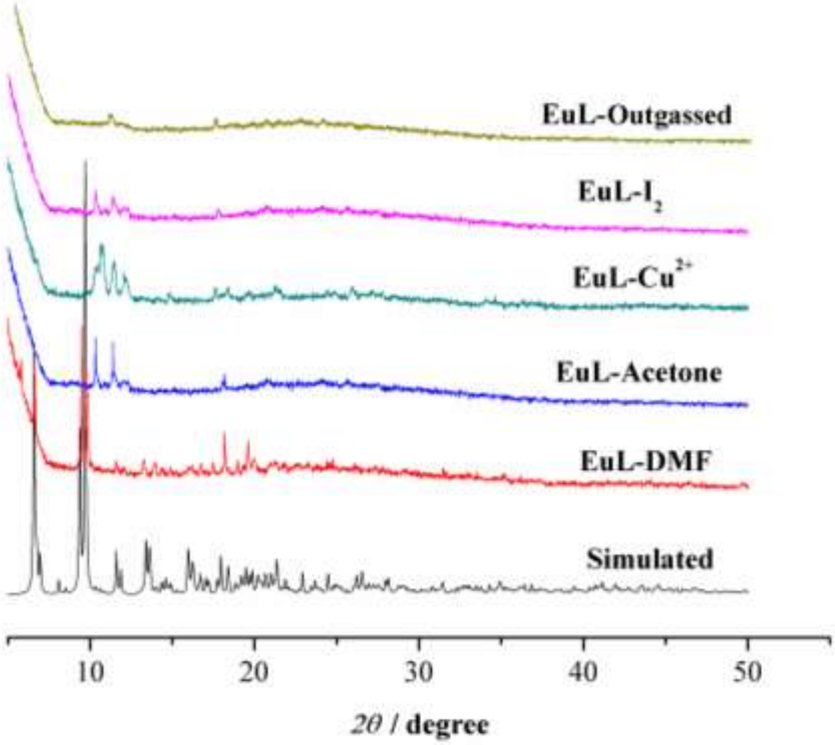

Table S1. Selected bond lengths (Å) and angles (º) for **EuL**.

	Bond Lengths (Å)		Bond Lengths (Å)
Eu(1)-O(25)	2.349(3)	Eu(1)-O(19)$^{\#1}$	2.373(3)
Eu(1)-O(20)	2.392(2)	Eu(1)-O(33)$^{\#2}$	2.418(3)
Eu(1)-O(21)	2.434(3)	Eu(1)-O(24)	2.471(3)
Eu(1)-O(23)	2.488(3)	Eu(1)-O(22)	2.489(3)
Eu(1)-O(25)$^{\#1}$	2.817(3)	Eu(2)-O(8)	2.316(3)
Eu(2)-O(15)	2.324(3)	Eu(2)-O(12)	2.328(3)
Eu(2)-O(14)	2.447(3)	Eu(2)-O(13)	2.457(4)
Eu(2)-O(9)	2.461(3)	Eu(2)-O(11)	2.469(3)
Eu(2)-O(10)	2.488(2)	Eu(3)-O(3)	2.311(3)
Eu(3)-O(2)	2.347(3)	Eu(3)-O(1)$^{\#3}$	2.404(2)
Eu(3)-O(7)	2.410(3)	Eu(3)-O(6)	2.430(3)
Eu(3)-O(4)	2.460(3)	Eu(3)-O(5)	2.467(3)
Eu(3)-O(34)$^{\#4}$	2.469(3)	Eu(4)-O(29)	2.293(3)
Eu(4)-O(31)	2.330(3)	Eu(4)-O(32)$^{\#5}$	2.345(3)
Eu(4)-O(26)	2.363(3)	Eu(4)-O(28)	2.472(3)
Eu(4)-O(18)	2.479(3)	Eu(4)-O(27)	2.489(3)
Eu(4)-O(17)	2.503(3)		
	Bond Angles (º)		Bond Angles (º)
O(25)-Eu(1)-O(19)$^{\#1}$	74.87(9)	O(19)$^{\#1}$-Eu(1)-O(20)	133.26(9)
O(25)-Eu(1)-O(21)	82.51(11)	O(20)-Eu(1)-O(24)	140.75(10)
O(19)$^{\#1}$-Eu(1)-O(23)	76.76(11)	O(25)-Eu(1)-O(22)	150.81(12)
O(21)-Eu(1)-O(22)	75.87(13)	O(33)$^{\#2}$-Eu(1)-O(25)$^{\#1}$	48.76(8)
O(21)-Eu(1)-O(25)$^{\#1}$	137.93(9)	O(22)-Eu(1)-O(25)$^{\#1}$	105.54(10)
O(15)-Eu(2)-O(12)	153.03(10)	O(8)-Eu(2)-O(14)	140.38(10)
O(8)-Eu(2)-O(13)	147.00(11)	O(12)-Eu(2)-O(13)	76.06(12)
O(14)-Eu(2)-O(9)	127.96(10)	O(13)-Eu(2)-O(9)	73.21(12)
O(13)-Eu(2)-O(11)	136.95(11)	O(9)-Eu(2)-O(11)	149.43(10)
O(12)-Eu(2)-O(10)	76.67(9)	O(11)-Eu(2)-O(10)	128.50(9)
O(2)-Eu(3)-O(1)$^{\#3}$	124.87(9)	O(1)$^{\#3}$-Eu(3)-O(7)	80.22(10)
O(2)-Eu(3)-O(6)	137.06(11)	O(2)-Eu(3)-O(4)	77.97(11)
O(6)-Eu(3)-O(4)	105.61(11)	O(3)-Eu(3)-O(5)	81.45(11)
O(2)-Eu(3)-O(5)	142.12(11)	O(4)-Eu(3)-O(5)	71.04(11)
O(3)-Eu(3)-O(34)$^{\#4}$	133.28(9)	O(7)-Eu(3)-O(34)$^{\#4}$	84.48(10)
O(29)-Eu(4)-O(31)	90.59(11)	O(29)-Eu(4)-O(32)$^{\#5}$	153.96(11)
O(29)-Eu(4)-O(26)	95.05(12)	O(31)-Eu(4)-O(26)	146.57(12)
O(32)$^{\#5}$-Eu(4)-O(28)	86.23(10)	O(26)-Eu(4)-O(28)	140.44(11)
O(31)-Eu(4)-O(18)	71.42(10)	O(26)-Eu(4)-O(27)	71.68(11)
O(18)-Eu(4)-O(27)	140.51(9)	O(27)-Eu(4)-O(17)	136.94(10)

Table S2. The intensity ratios ($R=I_2/I_1$) between the $^5D_0\rightarrow{}^7F_1$ and $^5D_0\rightarrow{}^7F_2$ transitions for **EuL** in different solvent molecules and metal ions. It is known that the transition $^5D_0\rightarrow{}^7F_1$ belongs to a magnetic dipolar transition that is insensitive to the surrounding environment of the Eu^{3+} ions, whereas $^5D_0\rightarrow{}^7F_2$ is an electric dipolar transition, and the relative intensity ratio (R) of $^5D_0\rightarrow{}^7F_1$ to $^5D_0\rightarrow{}^7F_2$ can indicate how far the local environment of the Eu^{3+} ions is centrosymmetric.[2] As calculated, the R values of samples are slightly different. Compared to the pure sample of **EuL**, Cu^{2+} ions have the greatest influence on the local environment of the Eu^{3+} ions.

	I_1 (intensity of $^5D_0\rightarrow{}^7F_1$)	I_2 (intensity of $^5D_0\rightarrow{}^7F_2$)	R ($R = I_2/I_1$)
Na^+	357	4660	13.05
Mg^{2+}	281	2308	8.21
Ni^{2+}	207	2146	10.37
Zn^{2+}	209	1594	7.63
Gd^{3+}	122	1773	14.53
Co^{2+}	78	937	12.01
Cu^{2+}	5.3	83	15.66
DMF	933	5592	5.99
ethanol	807	4680	5.80
methanol	587	3844	6.55
acetonitrile	567	3160	5.57
THF	662	3303	4.99
2-propanol	322	1807	5.61
acetone	13	147	11.31
Pure **EuL**	146	892	6.11

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