**Supporting information**

# Acid-induced Zn(II)-based metal-organic framework for encapsulation and sensitization of lanthanide cations

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## Table S1 Selected Distances and Bond Angles

| Compound **1** | | | |
|---|---|---|---|
| Zn(1)-O(3)#1 | 1.934(3) | Zn(2)-O(2)#4 | 2.045(3) |
| Zn(1)-O(7)#2 | 1.945(3) | Zn(2)-O(4)#1 | 2.076(4) |
| Zn(1)-O(1) | 1.947(3) | Zn(2)-O(4)#5 | 2.076(4) |
| Zn(1)-O(8)#3 | 1.972(3) | Zn(2)-O(9)#4 | 2.132(6) |
| Zn(2)-O(2) | 2.045(3) | Zn(2)-O(9) | 2.132(6) |
| O(1)-C(1) | 1.277(5) | O(5)-C(16) | 1.314(7) |
| O(2)-C(1) | 1.234(6) | O(6)-C(16) | 1.220(7) |
| O(3)-C(15) | 1.235(6) | O(7)-C(8) | 1.248(6) |
| O(4)-C(15) | 1.222(6) | O(8)-C(8) | 1.251(6) |
| | | | |
| O(3)#1-Zn(1)-O(7)#2 | 127.94(18) | O(4)#1-Zn(2)-O(4)#5 | 180.0 |
| O(3)#1-Zn(1)-O(1) | 117.37(17) | O(2)-Zn(2)-O(9)#4 | 90.21(16) |
| O(7)#2-Zn(1)-O(1) | 105.02(16) | O(2)#4-Zn(2)-O(9)#4 | 89.79(16) |
| O(3)#1-Zn(1)-O(8)#3 | 100.90(17) | O(4)#1-Zn(2)-O(9)#4 | 88.0(3) |
| O(7)#2-Zn(1)-O(8)#3 | 104.27(16) | O(4)#5-Zn(2)-O(9)#4 | 92.0(3) |
| O(1)-Zn(1)-O(8)#3 | 94.87(14) | O(2)-Zn(2)-O(9) | 89.79(16) |
| O(2)-Zn(2)-O(2)#4 | 180.0 | O(2)#4-Zn(2)-O(9) | 90.21(16) |
| O(2)-Zn(2)-O(4)#1 | 92.76(15) | O(4)#1-Zn(2)-O(9) | 92.0(3) |
| O(2)#4-Zn(2)-O(4)#1 | 87.24(15) | O(4)#5-Zn(2)-O(9) | 88.0(3) |
| O(2)-Zn(2)-O(4)#5 | 87.24(15) | O(9)#4-Zn(2)-O(9) | 180.0(4) |
| O(2)#4-Zn(2)-O(4)#5 | 92.76(15) | | |
| Compound **2** | | | |
| Zn(1)-O(3)#1 | 1.912(4) | Zn(2)-O(11)#3 | 1.978(5) |
| Zn(1)-O(8)#2 | 1.913(5) | Zn(3)-O(9)#4 | 1.978(6) |
| Zn(1)-O(12)#3 | 1.953(4) | Zn(3)-O(9)#2 | 1.978(6) |
| Zn(1)-O(1) | 1.987(4) | Zn(3)-O(13) | 2.035(15) |
| Zn(2)-O(5) | 1.914(4) | Zn(3)-O(6)#5 | 2.138(5) |
| Zn(2)-O(2) | 1.919(4) | Zn(3)-O(6) | 2.138(5) |
| Zn(2)-O(10)#4 | 1.947(4) | | |
| O(1)-C(1) | 1.246(7) | O(7)-C(22) | 1.227(8) |
| O(2)-C(1) | 1.256(7) | O(8)-C(22) | 1.245(8) |
| O(3)-C(8) | 1.249(8) | O(9)-C(23) | 1.270(9) |
| O(4)-C(8) | 1.208(8) | O(10)-C(23) | 1.226(8) |
| O(5)-C(9) | 1.281(7) | O(11)-C(24) | 1.233(7) |

| | | | |
|---|---|---|---|
| O(6)-C(9) | 1.238(7) | O(12)-C(24) | 1.252(7) |
| | | | |
| O(3)#1-Zn(1)-O(8)#2 | 115.4(2) | O(9)#2-Zn(3)-O(6)#5 | 95.1(2) |
| O(3)#1-Zn(1)-O(12)#3 | 109.7(2) | O(13)-Zn(3)-O(6)#5 | 87.27(15) |
| O(8)#2-Zn(1)-O(12)#3 | 122.1(2) | O(9)#4-Zn(3)-O(6) | 95.1(2) |
| O(3)#1-Zn(1)-O(1) | 95.26(19) | O(9)#2-Zn(3)-O(6) | 88.0(2) |
| O(8)#2-Zn(1)-O(1) | 99.7(2) | O(13)-Zn(3)-O(6) | 87.28(15) |
| O(12)#3-Zn(1)-O(1) | 110.55(19) | O(6)#5-Zn(3)-O(6) | 174.6(3) |
| O(5)-Zn(2)-O(2) | 123.7(2) | C(1)-O(1)-Zn(1) | 136.0(4) |
| O(5)-Zn(2)-O(10)#4 | 117.6(2) | C(1)-O(2)-Zn(2) | 130.6(4) |
| O(2)-Zn(2)-O(10)#4 | 106.4(2) | C(8)-O(3)-Zn(1)#1 | 126.9(4) |
| O(5)-Zn(2)-O(11)#3 | 103.7(2) | C(9)-O(5)-Zn(2) | 116.2(4) |
| O(2)-Zn(2)-O(11)#3 | 106.5(2) | C(9)-O(6)-Zn(3) | 142.4(4) |
| O(10)#4-Zn(2)-O(11)#3 | 94.06(19) | C(22)-O(8)-Zn(1)#2 | 125.5(4) |
| O(9)#4-Zn(3)-O(9)#2 | 109.3(5) | C(23)-O(9)-Zn(3)#2 | 143.6(7) |
| O(9)#4-Zn(3)-O(13) | 125.3(2) | C(23)-O(10)-Zn(2)#6 | 120.5(4) |
| O(9)#2-Zn(3)-O(13) | 125.3(2) | C(24)-O(11)-Zn(2)#3 | 147.4(4) |
| O(9)#4-Zn(3)-O(6)#5 | 88.0(2) | C(24)-O(12)-Zn(1)#3 | 123.0(4) |

Symmetry codes used for **1**: #1 x-1/2,-y+1/2,z-1/2; #2 x,-y,z-1/2; #3 -x,-y,-z+1; #4 -x+1/2,-y+1/2,-z+1; #5 -x+1,y,-z+3/2; **2**: #1 -x+1/2,-y+1/2,-z+1; #2 -x,-y,-z+1; #3 -x+1,-y,-z+1; #4 x,-y,z-1/2; #5 -x,y,-z+1/2; #6 x,-y,z+1/2.

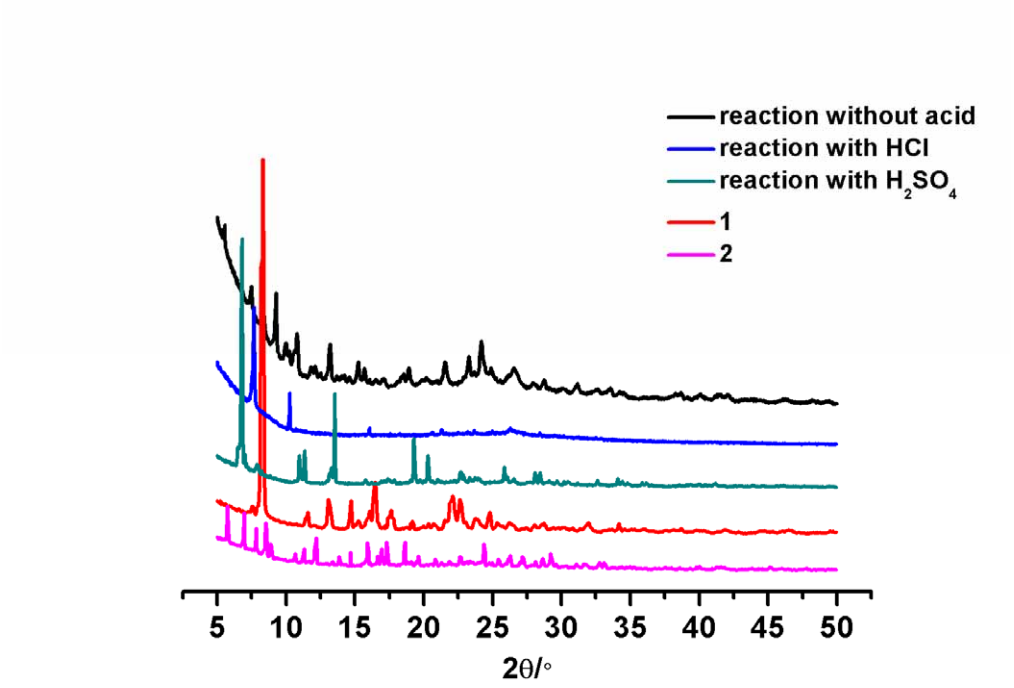


**Figure S1a** PXRD patterns of powders under the reaction using different acids and without acid, **1** and **2** are used for comparison

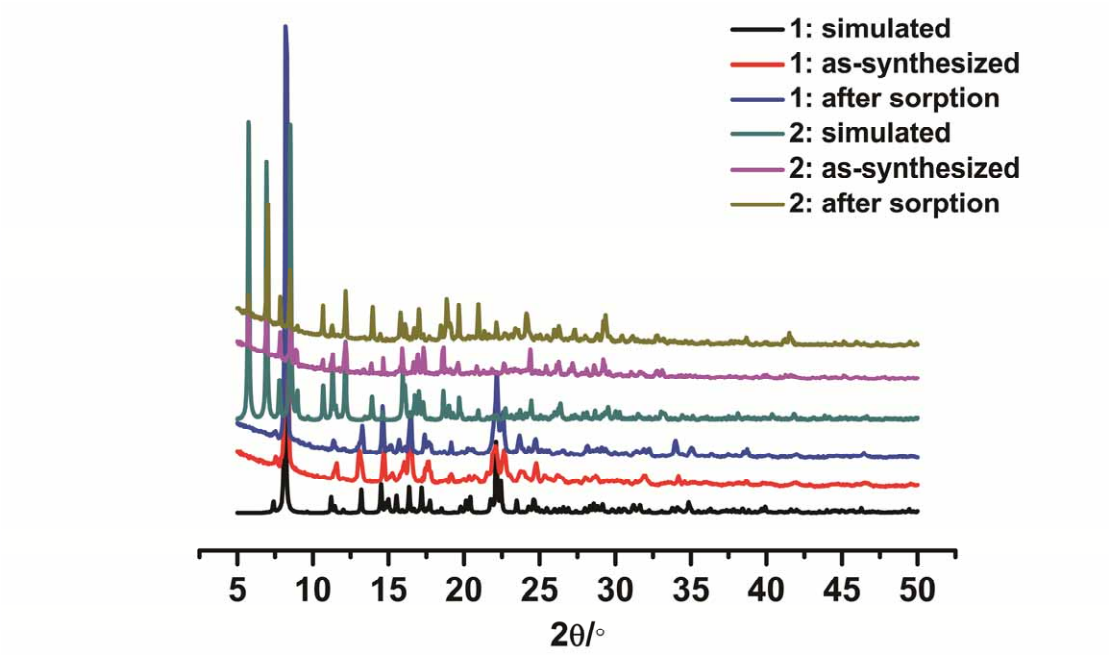


**Figure S1b** PXRD patterns of **1** and **2**: simulated, as-synthesized and after sorption

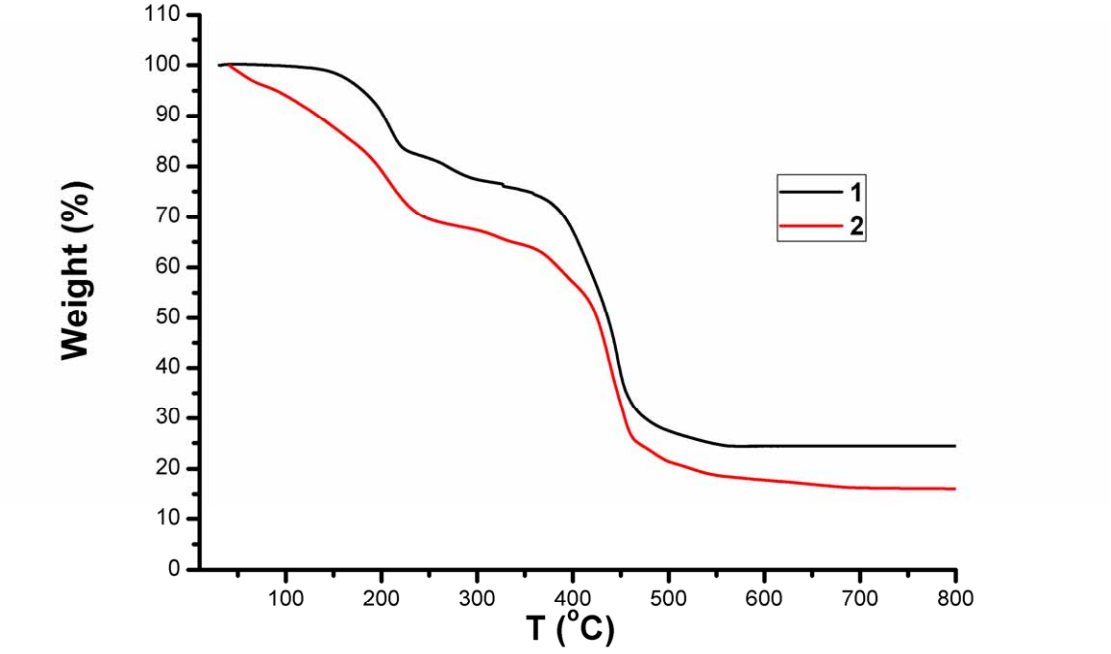


**Figure S2** TGA data of **1** and **2**

**Fig. S3** Photographs of samples **Cu@1** (left) and **1** (right)

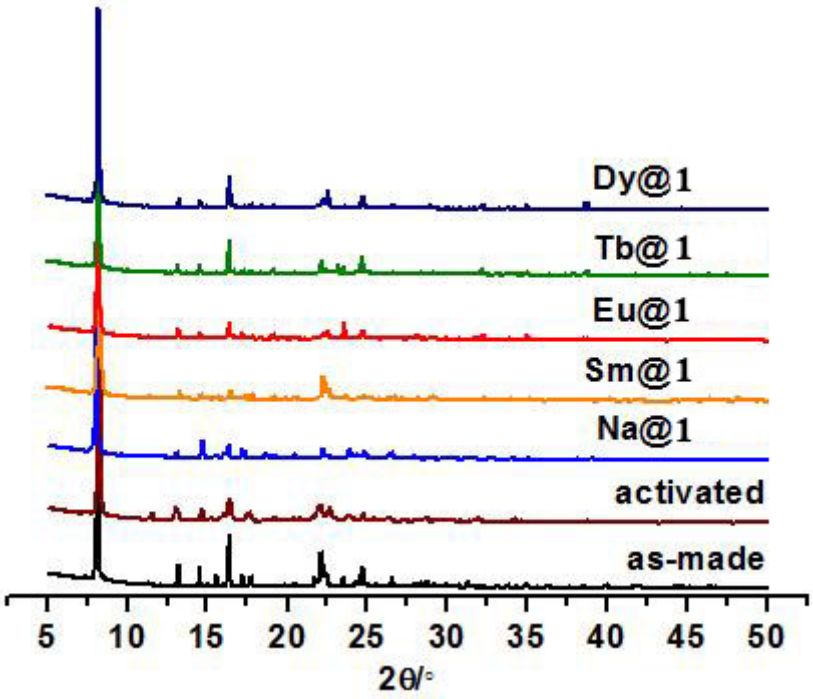


**Fig. S4** PXRD patterns of **1, Na@1** and **Ln@1**

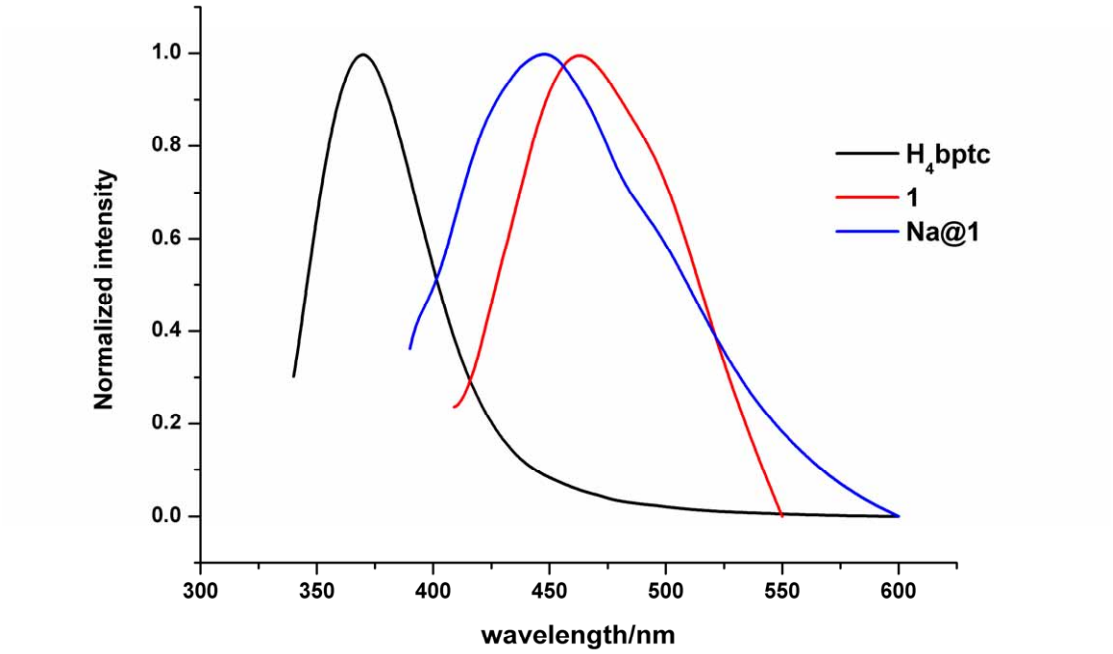


**Figure S5** Solid state luminescence spectra **of $H_4$bptc** excited at 316nm**, 1** excited at 385nm and **Na@1** excited at 365 nm**.**