Electronic Supplementary Information

Long-afterglow Metal-Organic Frameworks: Reversible Guest-induced Phosphorescence Tunability

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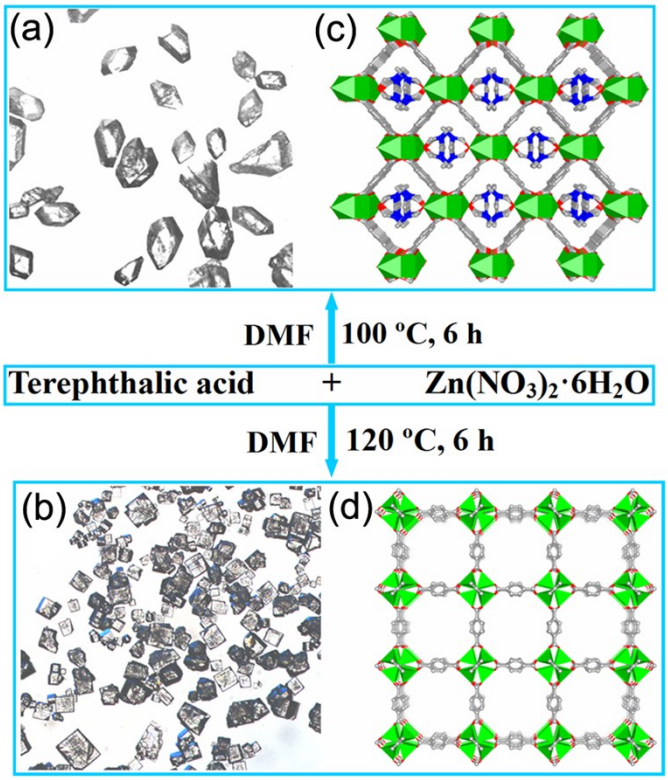


Figure S1. Scheme for synthesis of **1-DMF** (a) and **MOF-5** (b) single crystals; single crystal structure of **1-DMF** (c) and **MOF-5** (d). Hydrogen atoms have been omitted for clarity. C, grey; N, blue; O, red; Zn, green.

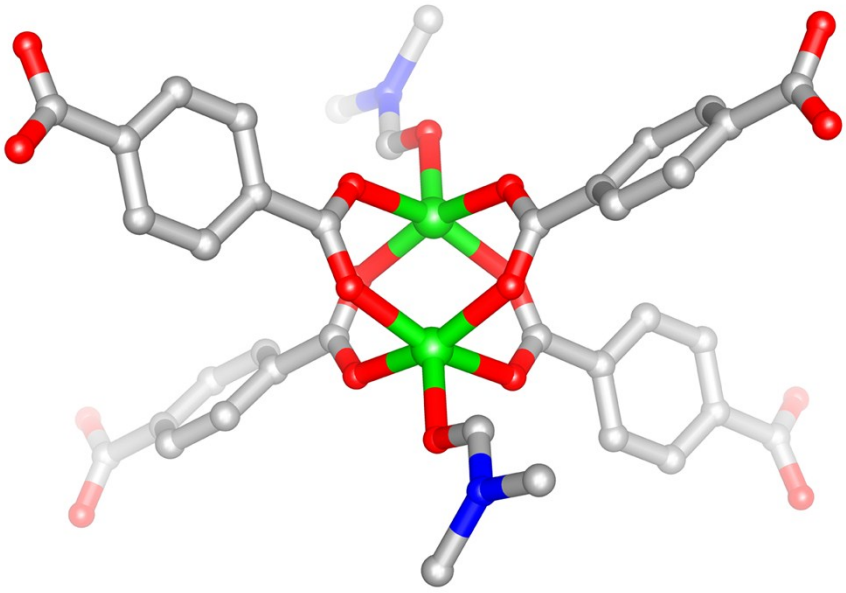
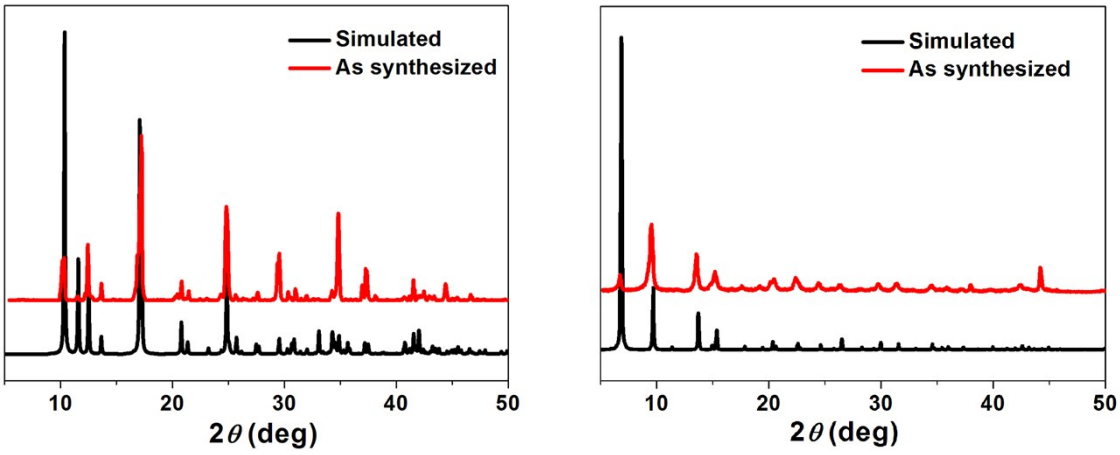
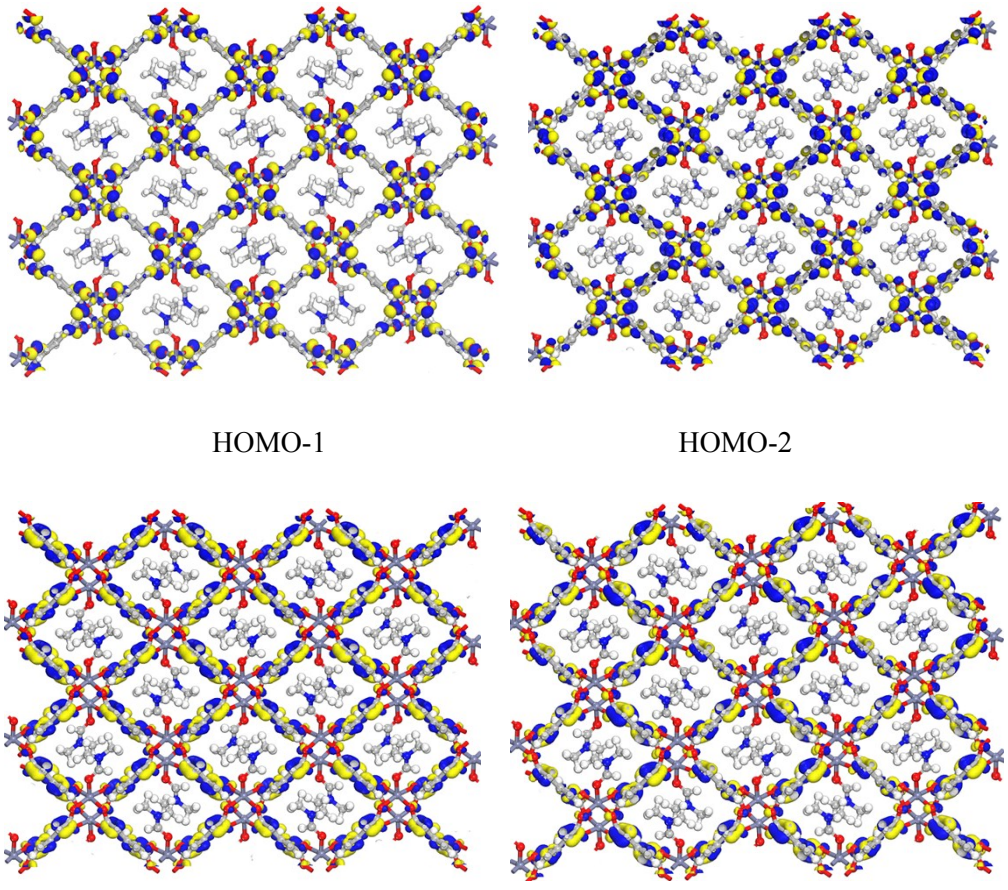


Figure S2. Ball-and-stick view of the paddle-wheel unit in **1-DMF**.



(a) (b)

Figure S3. Simulated and as synthesized PXRD patterns of **1-DMF** and **MOF-5**.



HOMO-1 HOMO-2

LUMO+1 LUMO+2

Figure S4. The electron-density distribution of various orbitals involved in **1-DMF**.

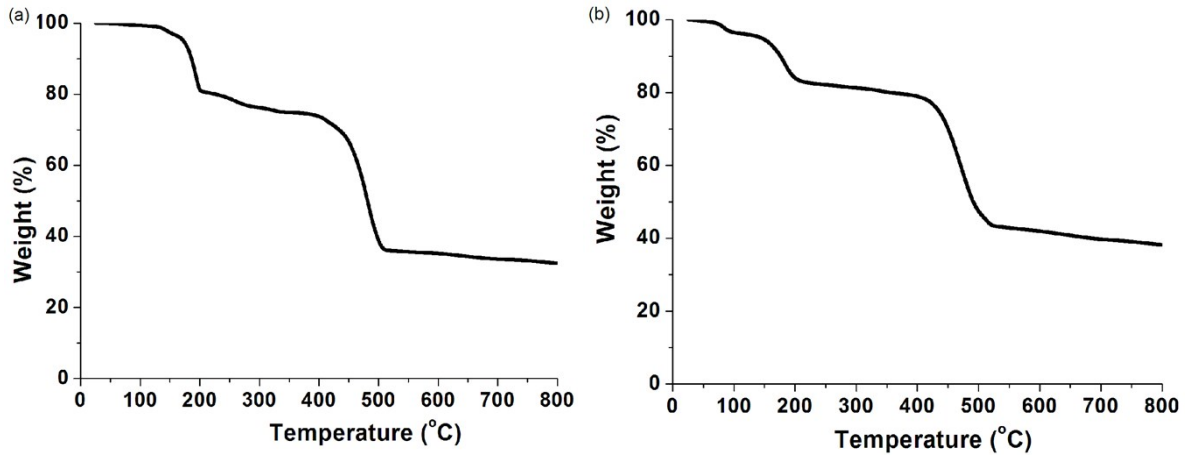


Figure S5. Thermogravimetric (TG) analysis curves of **1-DMF** (a) and **MOF-5** (b).

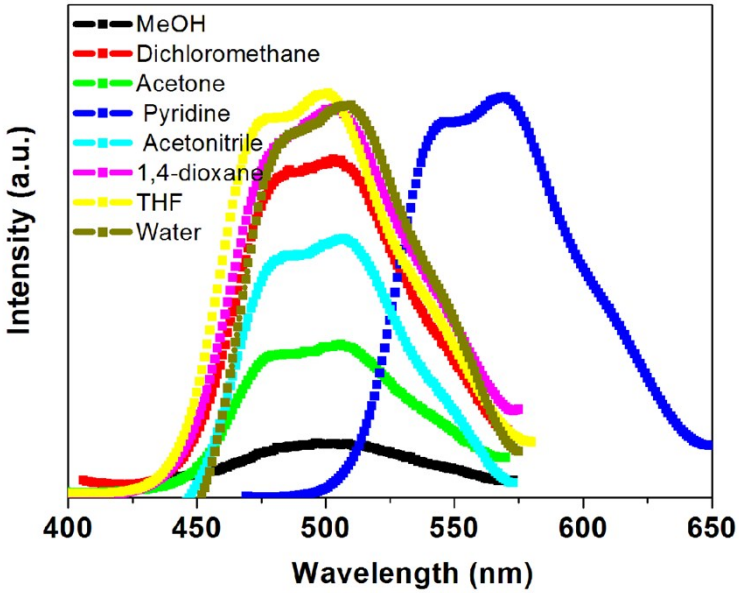


Figure S6. Phosphorescence spectra of **1-DMF** after immersing in different solvents.

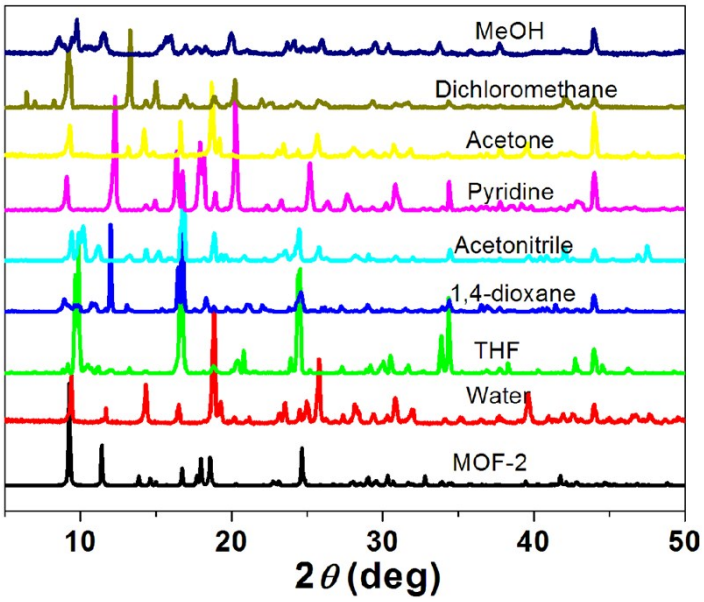
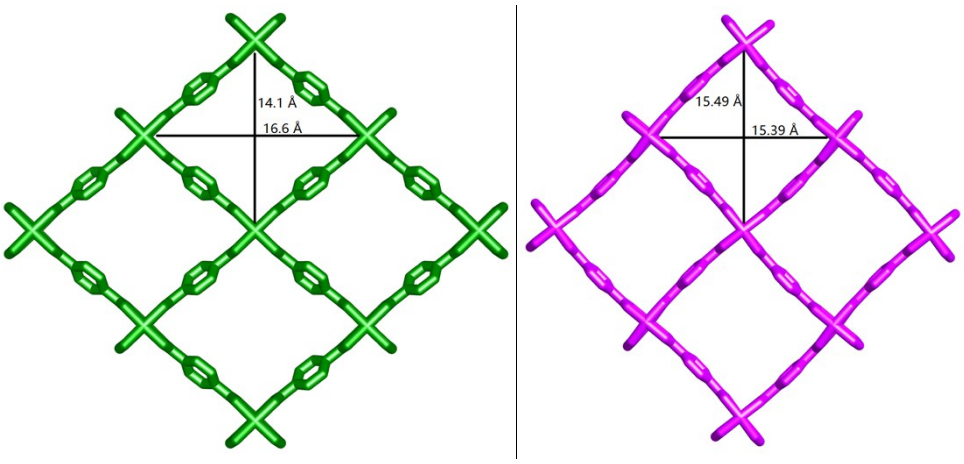


Figure S7. PXRD patterns of **MOF-2** and **1-DMF** after immersing in different solvents.



(a) (b)

Figure S8. View of the 2D layer for **1-DMF** (a) and **MOF-2** (b).

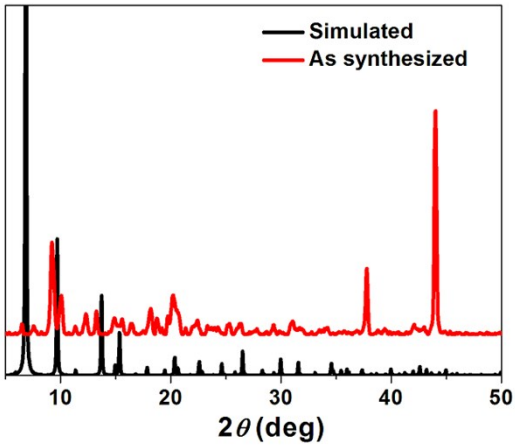


Figure S9. PXRD patterns of **MOF-5** treated with pyridine.

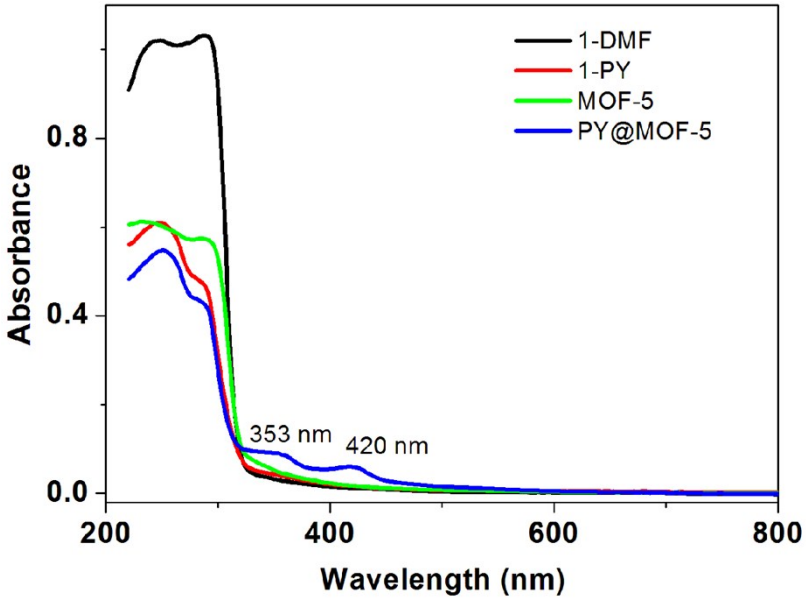


Figure S10. UV-visible absorption spectra for **1-DMF**and **MOF-5** and the samples after pyridine treatment.

Table S1. Crystallographic data for **1-DMF** [a].

Compound	**1-DMF**
Formula	$C_{11}H_6ZnNO_5$
Formula weight	297.54
Crystal system	Monoclinic
Space group	*C*2/*m*
a (Å)	11.191(6)
b (Å)	14.136(8)
c (Å)	7.975(5)
α (°)	90
β (°)	106.894(7)
γ (°)	90
V (Å^3)	1207.2(12)
Z	4
D_c (g/cm^3)	1.637
Abs. coeff. /mm^{-1}	2.045
F(000)	596
θ range for data collection (°)	2.39 / 25.49
GOF	1.236
R [$I > 2\sigma(I)$]	$R_1 = 0.0520$ $wR_2 = 0.1497$
R (all data)	$R_1 = 0.0532$ $wR_2 = 0.1501$

[a] $R = [\sum ||F_0| - |F_c|| / \sum |F_0|]$, $R_W = \sum_W [|F_0^2 - Fc^2|^2 / \sum_W (|F_w|^2)^2]^{1/2}$

Table S2. Selected bond lengths (Å) and angles (°) for **1-DMF**.

Zn(1)-O(3)	1.988(7)	Zn(1)-O(2)#1	2.017(5)
Zn(1)-O(2)#2	2.017(5)	Zn(1)-O(1)	2.037(5)
Zn(1)-O(1)#3	2.037(5)		
O(3)-Zn(1)-O(2)#1	103.4(2)	O(3)-Zn(1)-O(2)#2	103.4(2)
O(2)#1-Zn(1)-O(2)#2	85.6(3)	O(3)-Zn(1)-O(1)	97.2(2)
O(2)#1-Zn(1)-O(1)	159.4(2)	O(2)#2-Zn(1)-O(1)	89.7(2)
O(3)-Zn(1)-O(1)#3	97.2(2)	O(2)#1-Zn(1)-O(1)#3	89.7(2)
O(2)#2-Zn(1)-O(1)#3	159.4(2)	O(1)-Zn(1)-O(1)#3	87.7(4)

[a]Symmetry codes for **1-DMF**: #1 -*x*, *y*, -*z* + 1; #2 -*x*, -*y*, -*z* + 1; #3 *x*, -*y*, *z*.

Table S3. The cell parameter comparison of **1-DMF** and **MOF-2**.

Parameter	**1-DMF**	**MOF-2**
Crystal system	Monoclinic	Monoclinic
Space group	*C*2/*m*	$P2_1/n$
a (Å)	11.191(6)	6.718 (3)
b (Å)	14.136(8)	15.488(7)
c (Å)	7.975(5)	12.430(8)
β (°)	106.894(7)	102.83(4)
V (Å^3)	1207.2(12)	1261.0 (11)