Supplementary Information (SI)

A series of naphthalenediimide-based metal-organic frameworks: synthesis, photochromism and inkless and erasable printing

Xiao-Feng Zhong,^a Guo-Jun Luo,^a Wen-Bin Li,^a Xiong-Hai Chen,^a Ying Wu,^a Yi-Hui Chen,^a Jia-Wen Ye, Jie Bai,^b Zong-Wen Mo,^{*a} and Xiao-Ming Chen^{ac}

^a School of Biotechnology and Health Sciences, Wuyi University, Jiangmen, Guangdong 529020, PR China.

^b Analysis and Test Center, Guangdong University of Technology, Guangzhou 510006, China.

^c MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry, Sun Yat-Sen University, Guangzhou 510275, China.

*Email: wyuchemmzw@126.com



Fig. S1. Perspective views of the asymmetric unit of **1** (symmetry codes: A = x, 1+y, 1+z, B = 2-x, 1+y, 3/2-z, C = 1/2+x, 3/2-y, 1/2+z, D = 1/2+x, 1/2+y, 1+z).



Fig. S2 The pore surface of 1.



Fig. S3. Perspective views of the asymmetric unit of **2** (symmetry codes: A = 1-x, 1-y, 1-z, B = x, y, z, C = 1-x, 1-y, -z, D = -x, -y, 1-z, E = 1+x, y, -1+z, F = 1+x, y, z, G = 2+x, 1+y, -1+z,).



Fig. S4. The pore surface of 2.



Fig. S5. Perspective views of the asymmetric unit of **3** (symmetry codes: A = 1-x, 2-*y*, 2-*z*, B = x, 1+y, 2+z, C = -1+x, 1+y, 2+z, D = -x, 2-*y*, 2-*z*, E = -1+x, *y*, *z*).



Fig. S6. The pore surface of 3.



Fig. S7. Thermogravimetric curves of 1-3.



Fig. S8. PXRD patterns of 1 under different treatments.



Fig. S9. PXRD patterns of 2 under different treatments.



Fig. S10. PXRD patterns of 3 under different treatments.



Fig. S11. The colour change of H₄BINDI under UV light (365 nm)/visible light and dark.



Fig. S12. EPR spectra for H₄BINDI before and after irradiation.



Fig. S13. SEM images of the surface (a) and cross section (b) of 2-coated paper.



Fig. S14. SEM images of the surface (a) and cross section (b) of 3-coated paper.



Fig. S15. The resolution test of 2 by printing vertical lines with different widths.



Fig. S16. The resolution test of 3 by printing vertical lines with different widths.



Fig. S17. Printed content of the 2-coated paper at different times and the cycle test.



Fig. S18. Mechanical deformation test for the 2-coated paper.



Fig. S19. Mechanical deformation test for the 3-coated paper.



Fig. S20. FT-IR spectra for 1 and 1a.



Fig. S21. FT-IR spectra for 2 and 2a.



Fig. S22. FT-IR spectra for 3 and 3a.



Fig. S23. 2 and 3 Photochromic after exchange of different solvents.

	1	2	3
Elemental Analysis	3 H ₂ O + 6.5 DMF	14 H ₂ O + 3.7 DMF	2.5 H ₂ O + 0.5 DMF
Thermogravimetric Analysis	3 H ₂ O + 6.5 DMF +10 EtOH	0.8 DMF	4 H ₂ O + 1 DMF
Refinement and Squeeze Guset	3 H ₂ O + 6.5 DMF	2 DMF	2.5 H ₂ O + 0.5 DMF

Table S1. The possible content of guest molecular under different measurement.

Complex	1	2	3
Formula	$C_{33}H_{20}La_1N_3O_{14}{\cdot}3H_2O{\cdot}6.5$	$C_{72}H_{52}La_2N_8O_{29}{\cdot}2C_3H_7N$	$C_{47.25}H_{34.75}La_2N_{3.75}O_{26}{\cdot}2.5$
	C ₃ H ₇ NO	О	$H_2O \cdot 0.5C_3H_7NO$
Formula weight	1350.60	1917.22	1430.44
Temperature (K)	298(2)	298(2)	298(2)
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	C2/c	<i>P</i> -1	<i>P</i> -1
a/Å	35.8643(9)	14.8023(4)	10.31370(10)
$b/{ m \AA}$	22.9736(11)	15.7594(4)	13.1982(2)
$c/{ m \AA}$	17.0163(6)	18.6831(4)	19.8651(2)
$lpha/^{ m o}$	90	104.480(2)	89.5480(10)
$eta / ^{ m o}$	92.965(3)	97.442(2)	83.4300(10)
$\gamma^{\prime o}$	90	95.258(2)	74.6130(10)
$V/\text{\AA}^3$	14001.5(9)	4149.26(18)	2589.32(5)
Ζ	8	2	2
$D_{\rm c}/{ m g~cm^{-3}}$	1.281	1.535	1.730
reflns coll.	8303	14048	9213
unique reflns	12308	16771	10456
$R_{ m int}$	0.0746	0.0660	0.0423
$R_1 [I > 2\sigma(I)]^a$	0.0771	0.0523	0.0385
$wR_2[I > 2\sigma(I)]^b$	0.2119	0.1406	0.1064
R_1 (all data)	0.0952	0.0610	0.0431
wR_2 (all data)	0.2292	0.1480	0.1098
GOF	0.957	1.072	1.082

 Table S2. Crystallographic data and structural refinement detail of 1-3.

 ${}^{a}R_{1} = \Sigma ||F_{o}| - |F_{c}|| / \Sigma |F_{o}|.$

 ${}^{b}wR_{2} = \{ \Sigma w[(F_{o})^{2} - (F_{c})^{2}]^{2} / \Sigma w[(F_{o})^{2}]^{2} \}^{1/2}$