Supplementary Information

Structural elucidation and supercapacitive performance on a Mn(II)-based MOF

Chao Feng,[a, b, c] Chang-Peng Lv,[b, c] Hong Zhao,*[a] Zong-Qun Li,[b, c] Wei-Nan Xie,[a] Li-Na Sun,[a]

Yucheng Wang *[d]

[a] *School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, PR China. E-mail: zhaohong@seu.edu.cn*
[b] *Anhui Provincial Engineering Laboratory of Silicon-based Materials, Bengbu University, Bengbu 233030, PR China.*
[c] *Engineering Technology Research Center of Silicon-based Materials, Anhui Province, Bengbu University, Bengbu 233030, PR China.*
[d] *Institute of Medicinal Biotechnology, Chinese Academy of Medical Science and Peking Union Medical College, Beijing, 100050, PR China.*

Table S1 Crystal data and structure refinement parameters for the complex **1**

Complex	**1**
Empirical formular	$C_8H_6MnN_4O_4$
Formula weight	277.11
Crystal size/mm^3	0.3 x 0.25 x 0.22
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	*Fdd*2
a / Å	11.8741(7)
b / Å	18.4501(9)
c / Å	8.0067 (4)
V / Å^3	1754.09 (16)
Z	8
D_{calc} /g·cm^{-3}	2.099
μ/ mm^{-1}	1.516
θ range/°	4.1 to 25.0
Reflections collected	1793
Independent reflections	683
Observed reflections	669
F(000)	1112
Data/restraints/parameters	683/180
Goodness-of-fit on F^2	1.08
R(all data)	R_1 = 0.0188, wR_2 = 0.0395
R indexes [$I>2\sigma(I)$]	R_1 = 0 .0178, wR_2 = 0.0385
Largest diff. peak and hole/e·Å^{-3}	0.17 and -0.19

Table S2 Selected bond distances (Å) and angles (°) for complex **1**

1			
Mn1—O1[a]	2.1312 (15)	Mn1—O2[b]	2.2012 (17)
Mn1—O1	2.1312 (15)	Mn1—O2[c]	2.2012 (17)
Mn1—N1[d]	2.264 (2)	Mn1—N14	2.264 (2)
O1[a]—Mn1—O1	175.94 (11)	O1—Mn1—O2[c]	94.09 (7)
O1[a]—Mn1—O2[b]	94.09 (7)	O2[a]—Mn1—O2[c]	96.80 (9)
O1—Mn1—O2[b]	88.60 (7)	O1[i]—Mn1—N1[d]	88.39 (7)
O1[a]—Mn1—O2[c]	88.60 (7)	O1—Mn1—N1[d]	88.65 (7)
O2[b]—Mn1—N1[d]	174.15 (8)	O2[b]—Mn1—N1[e]	88.55 (6)
O2[c]—Mn1—N1[d]	88.55 (6)	O2[c]—Mn1—N1[e]	174.15 (8)
O1[a]—Mn1—N1[e]	88.65 (7)	N1[d]—Mn1—N1[e]	86.22 (10)
O1—Mn1—N1[e]	88.39 (7)		

Symmetry code: (a) 7/4−*x*, −1/4+*y*, −1/4+*z*; (b) 2−*x*, 2−*y*, *z*.

Table S3 Pristine MOFs used as electrode materials

Order	MOFs	Electrolyte	Specific capacitance(F/g)	Refs.
1	MIL-100	0.1 M Na_2SO_4	34	S1
2	Co-MOF	1 M LiOH	206	S2
3	UIO-66	6 M KOH	207	S3
4	Ni-BCD	3 M KOH	998	S4
5	Ni-MOF	1 M KOH	184	S5
6	Ni- MOF	Alkali	1127	S6
7	$Ni_3(HITP)_2$	1 M $TEABF_4$/ACN	111	S7
8	Cd-pza	6 M KOH	106	S8
9	Co-MOF	5 M KOH	2564	S9
10	Mn-MOF	6 M KOH	443	This work

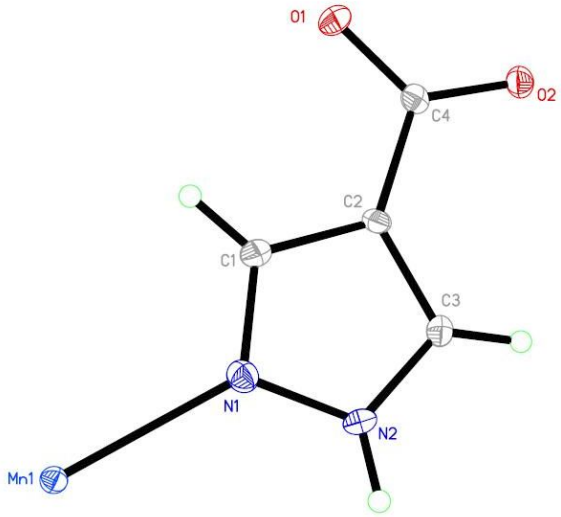

Figure S1 The asymmetry of **1** with thermal ellipse at the 30% probability level.

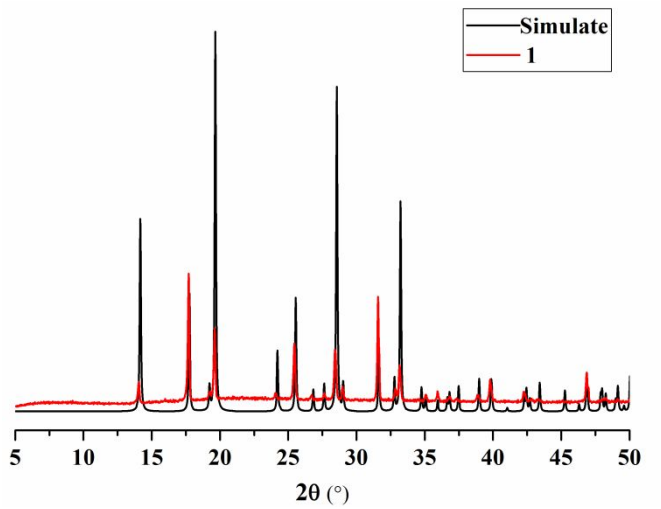

Figure S2 The XRD patterns of **1**

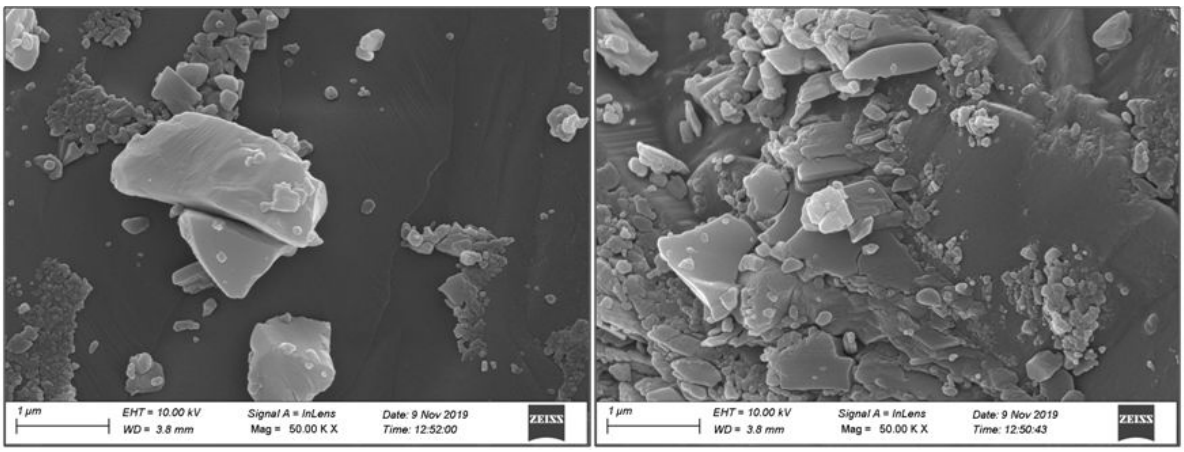

Figure S3 SEM images of the 3D network structure.

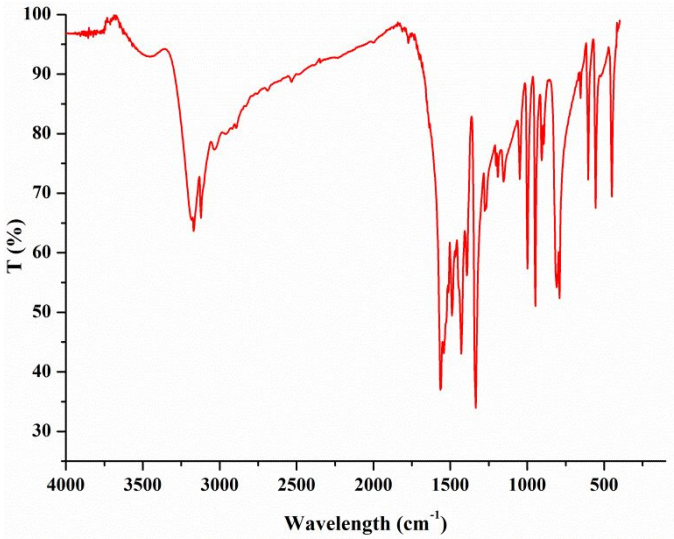

Figure S4 FT-IR of MOF **1**

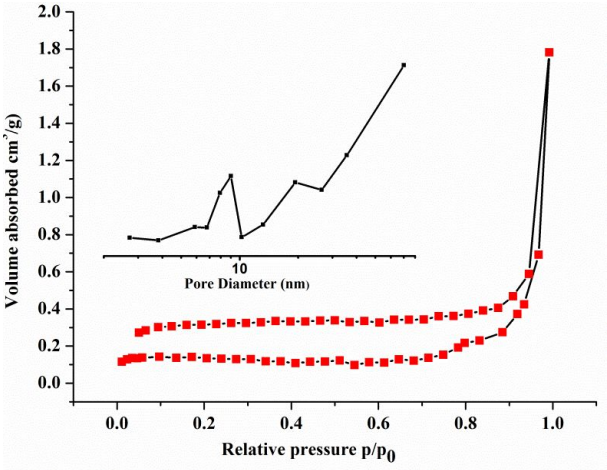

Figure S5 N_2 adsorption/desorption analysis isotherms at 77 K and pore size distribution on **1**

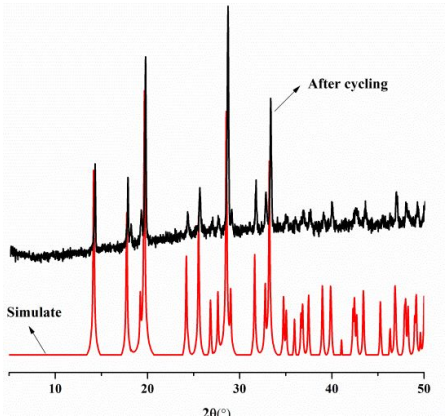

Figure S6 The PXRD of MOF **1** after cycling

Reference

S1. Campagnol, N.; Romero-Vara, R.; Deleu, W.; Stappers, L.; Binnemans, K.; De Vos D. E.;

Fransaer J. A hybrid supercapacitor based on porous carbon and the metal-organic framework MIL-100 (Fe). *ChemElectroChem* **2014**, *1*, 1182–1188.

S2. Lee, D. Y.; Yoon, S. J.; Shrestha, N. K.; Lee, S. H.; Ahn, H.; Han, S. H. Unusual energy storage and charge retention in Co-based metal–organic-frameworks. *Micropor. Mesopor. Mat.* **2012**, *153*, 163–165.

S3. Tan, Y.; Zhang, W.; Gao, Y.; Wu J.; Tang, B. Facile synthesis and supercapacitive properties of Zr-metal organic frameworks (UiO-66). *RSC Adv*. **2015**, *5*, 17601–17605.

S4. Yan, Y.; Gu, P.; Zheng, S.; Zheng, M.; Pang H.; Xue, H. Facile synthesis of an accordion-like Ni-MOF superstructure for high-performance flexible supercapacitors. *J. Mater. Chem. A* **2016**, *4*, 19078–19085.

S5. Feng, C.; Lv, C. P.; Li, Z. Q.; Zhao H.; Huang, H. H. A porous 2D Ni-MOF material with a high supercapacitive performance. *J. Solid State Chem*. **2018**, *265*, 244–247.

S6. Yang, J.; Xiong, P.; Zheng, C.; Qiu, H.; Wei, M. Metal–organic frameworks: a new promising class of materials for a high performance supercapacitor electrode. *J. Mater. Chem. A* **2014** , *2*,16640–16644.

S7. Wiktor, C.; Meledina, M.; Turner, S.; Lebedev, O. I.; Fischer, R. A. Transmission electron microscopy on metal–organic frameworks–a review. *J. Mater. Chem. A*. **2017**, *5*, 14969-14989.

S8. Feng, C.; Zhang, G. N.; Lv, C. P.; Jin, X. Q.; Sun, L. N. Structural elucidation and supercapacitive performance in a 1D cadmium(II) polymer based on pyrazole carboxylic acid. *J. Inorg. Organomet. Polym*. **2019**, *29*, 1559–1564.

S9. Yang, J.; Ma, Z.; Gao, W.; Wei, M. Layered structural Co-based MOF with conductive network frames as a new supercapacitor electrode. *Chem. Eur. J*. **2016**, *23*, 631–636.