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Supporting Information

Selective carbon dioxide sorption by a new breathing three-dimensional Zn-MOF with Lewis basic nitrogen-rich channels

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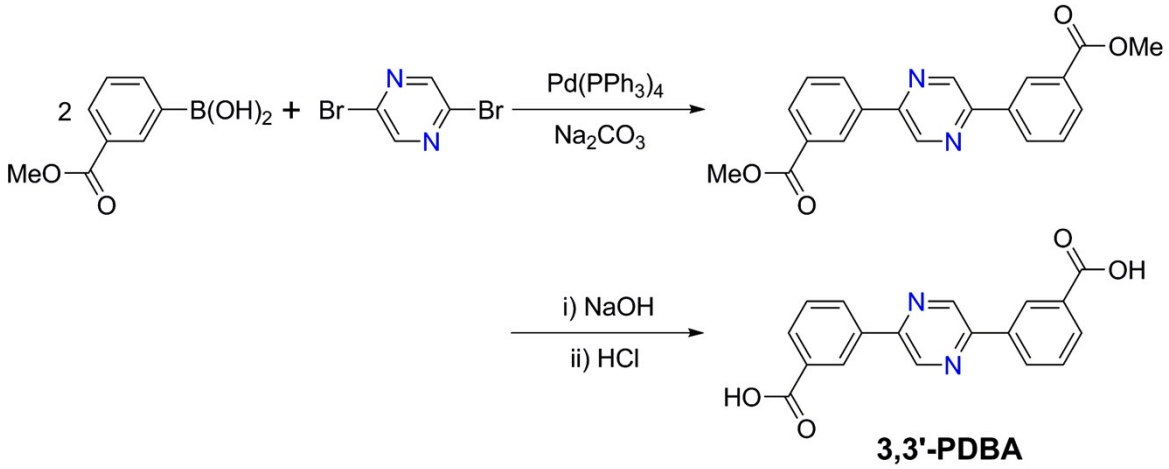

Figure S1. Preparation scheme for the new C_{2h}-symmetric 3,3'-PDBA bridging ligand by catalytic Suzuki coupling reaction.

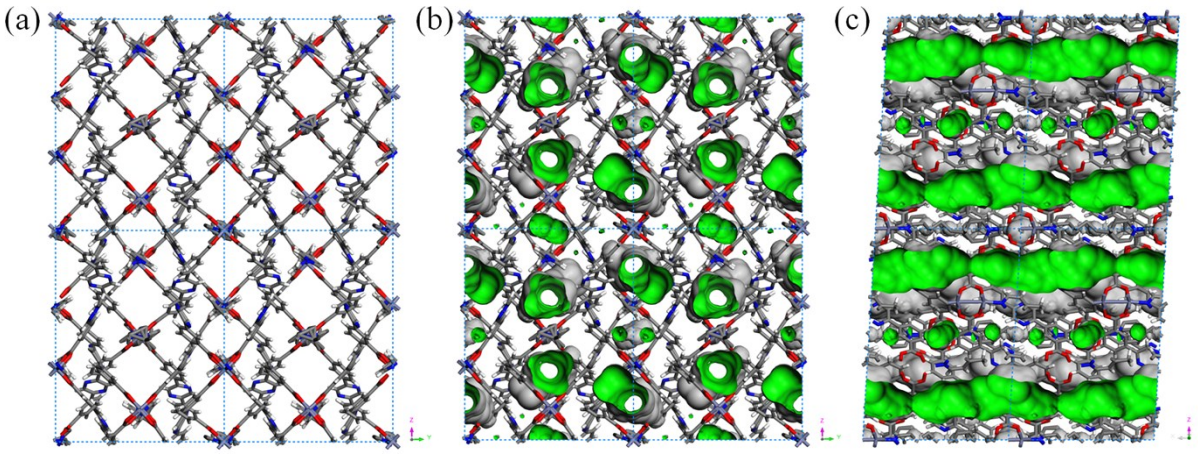

Figure S2. The framework of solvent-free Zn-MOF **1** shown along the *a*-axis (a), the corresponding Connolly surface (b), and the Connolly surface viewed down the *b*-axis (c) (Probe radius = 1.4 Å, Materials Studio 4.4).

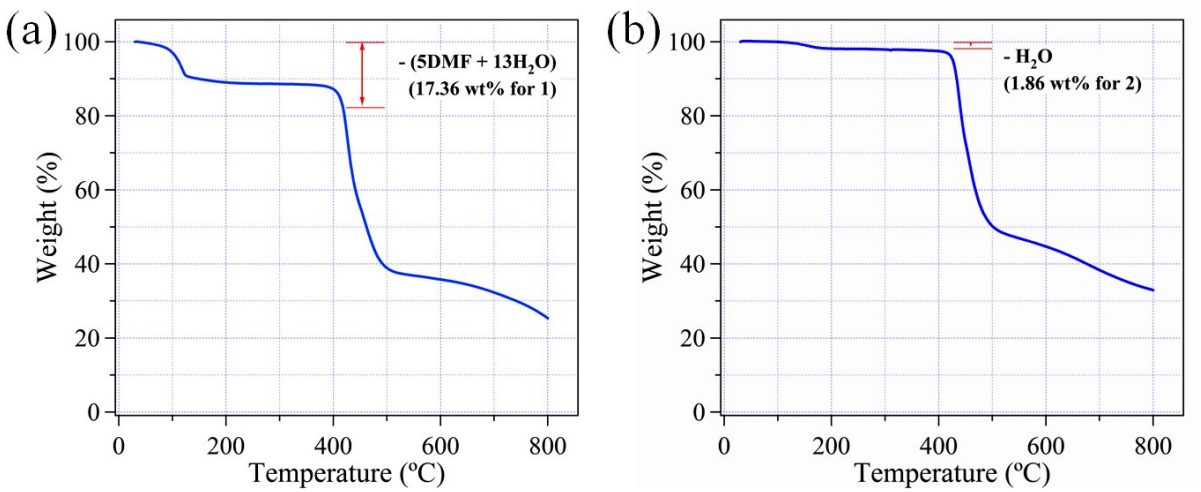

Figure S3. TG profiles of as-prepared Zn-MOF **1** (a) and Zn-MOF **2** (b) under continuous flow of nitrogen gas.

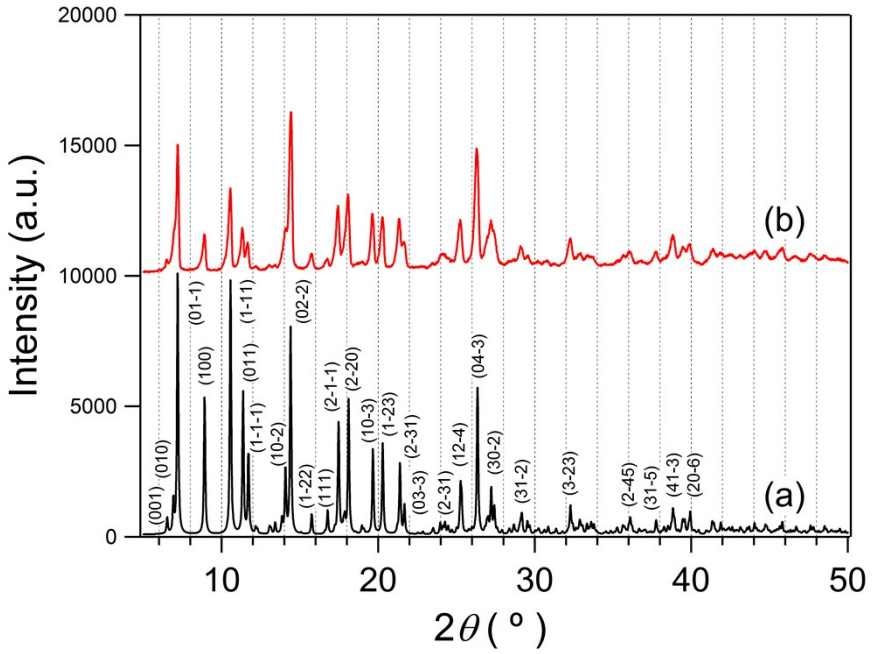

Figure S4. The PXRD pattern for Zn-MOF **2**. The simulated pattern from X-ray data (a) and the pattern for as-prepared sample (b).

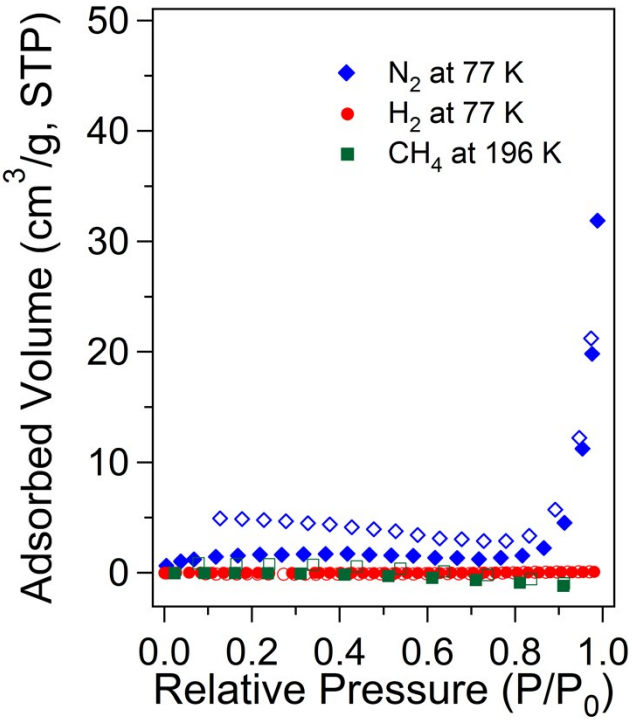

Figure S5. The adsorption/desorption isotherms of the activated Zn-MOF **1** for N_2, H_2, and CH_4. Solid symbols and open symbols represent adsorption and desorption isotherms, respectively.

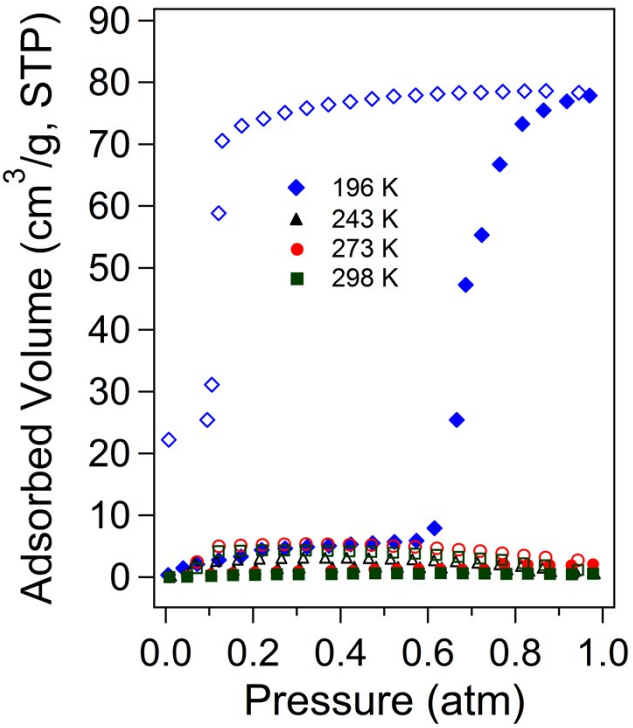

Figure S6. The adsorption/desorption isotherms of the activated Zn-MOF **1** for CO_2 at 196, 243, 273, and 298 K. Solid symbols and open symbols represent adsorption and desorption isotherms, respectively.

ToposPro analysis for Zn-MOF **1**

```
######################
1:C153 H68 N21 O27 Zn6
######################

Structure consists of 3D framework with FeVTiSc
There are 2 interpenetrating nets
FISE: Full interpenetration symmetry elements
-----------------------------------------------
1: -1
-----------------------------------------------
PIC: [1,0,0][0,0,1][0,1,0] (PICVR=1)

Zt=1; Zn=2

Class IIa  Z=2
Topology for Co1
--------------------
Atom Co1 links by bridge ligands and has
Common vertex with                    R(A-A)       f
Co 1   -1.0000    0.0000    0.0000   (-1 0 0)    16.255A       1
Co 1    1.0000    0.0000    0.0000   ( 1 0 0)    16.255A       1
Co 1    0.5000   -0.5000    0.5000   ( 0-1 0)    16.791A       1
Co 1   -0.5000    0.5000   -0.5000   (-1 0-1)    16.791A       1
Co 1   -0.5000   -0.5000   -0.5000   (-1-1-1)    16.791A       1
Co 1    0.5000    0.5000    0.5000   ( 0 0 0)    16.791A       1
-------------------------
Structural group analysis
-------------------------

-------------------------
Structural group No 1
-------------------------
Structure consists of 3D framework with NiCoCr2

Coordination sequences
----------------------
Co1:  1  2  3   4   5   6   7   8    9   10
Num   6 18 38  66 102 146 198 258  326  402
Cum   7 25 63 129 231 377 575 833 1159 1561
----------------------
TD10=1561

Vertex symbols for selected sublattice
---------------------------------------
Co1 Point symbol:{4^12.6^3}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]
---------------------------------------
Point symbol for net: {4^12.6^3}
6-c net; uninodal net

Topological type: pcu alpha-Po primitive cubic; 6/4/c1; sqc1 (topos&RCSR.ttd) {4^12.6^3} - VS
[4.4.4.4.4.4.4.4.4.4.4.*.*.*] (17092 types in 3 databases)
Elapsed time: 1.50 sec.
```

ToposPro analysis for Zn-MOF **2**

```
###################
1:C48 H30 N6 O8 Zn2
###################

Topology for V1
--------------------
Atom V1 links by bridge ligands and has
Common vertex with                    R(A-A)       f
V  1   -0.9745   -0.7268   -0.7232   (-1-1-1)    16.354A       1
V  1    1.0255    1.2732    1.2768   ( 1 1 1)    16.354A       1
Common edge with                      R(A-A)
V  1    0.0255    0.2732    1.2768   ( 0 0 1)    15.046A       2
V  1    0.0255    0.2732   -0.7232   ( 0 0-1)    15.046A       2
-------------------------
Structural group analysis
-------------------------

-------------------------
Structural group No 1
-------------------------
Structure consists of plane layers ( 1-1 0) with VTiSc2
Num. groups=2; Thickness=4.00; Min.Distance=4.846

Coordination sequences
----------------------
V1:  1  2  3  4  5  6   7   8   9  10
Num  4  8 12 16 20 24  28  32  36  40
Cum  5 13 25 41 61 85 113 145 181 221
----------------------
TD10=221

Vertex symbols for selected sublattice
---------------------------------------
V1 Point symbol:{4^4.6^2}
Extended point symbol:[4.4.4.4.6(2).6(2)]
---------------------------------------
Point symbol for net: {4^4.6^2}
4-c net; uninodal net
You have to increase Max.Ring value to compute plane net VS correctly!

Topological type: sql/Shubnikov tetragonal plane net (topos&RCSR.ttd) {4^4.6^2} - VS [4.4.4.4.*.*] (17092 types in 3 databases)
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```