Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Effect of Diol Isomers/Water Mixtures on the Stability of Zn-MOF-74

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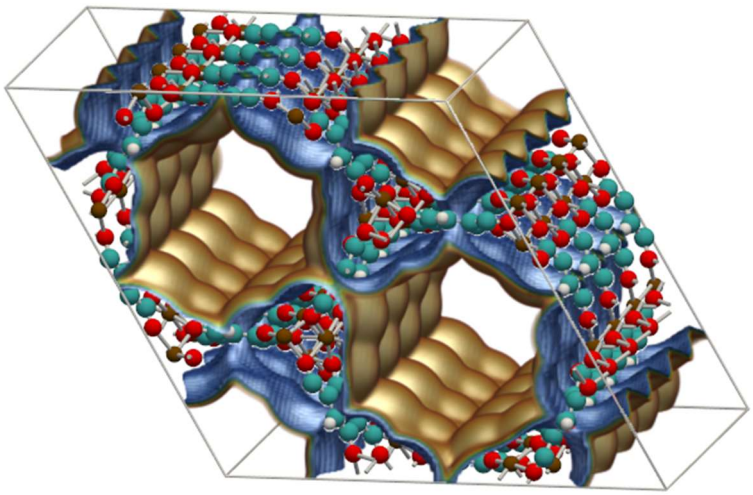

Figure S1. *Structure of Zn-MOF-74 with the Carbon atom in blue, the Hydrogen atom in white, the Oxygen atom in red and the metallic centre (Zn) in brown*.

Code S2. *Input used to carry out energy minimizations using LAMMPS code*.

```
#
units real
boundary p p p
atom_style full
pair_style reax/c NULL
pair_modify tail yes
box tilt large
read_data p1.data
# Pair potentials
pair_coeff * * Han.reax C C H H O Zn O O O C
# Recalculate charges
fix qeq_thermo all qeq/reax 1 0.0 10.0 1e-6 reax/c
# Minimisation Step:
minimize 1.0e-10 1.0e-10 1000 1000
unfix qeq_thermo
#
```

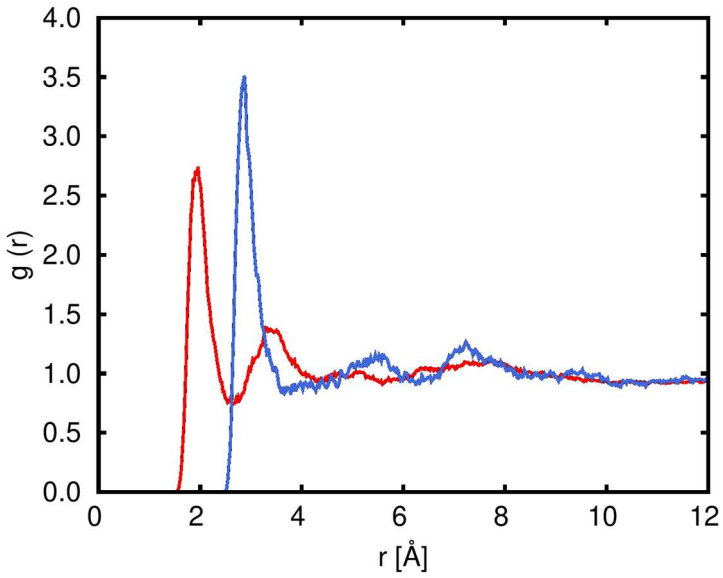

Figure S3. *Radial distribution functions of the oxygen of the molecules (blue) and the oxygen and hydrogen of the molecules (red).*

Equation S1. *Pore condensation degree*.

$$c(n_1, n_2, n_3) = \frac{3}{N\sqrt{6}} \cdot \sqrt{(\bar{n} - n_1)^2 + (\bar{n} - n_2)^2 + (\bar{n} - n_3)^2}$$

In this equation,

$c(n_1, n_2, n_3)$: pore condensation degree

N: total number of molecules

$\bar{n}$: average number of molecules per pore

n_i: number of molecules for each pore (*i=1,2,3*)

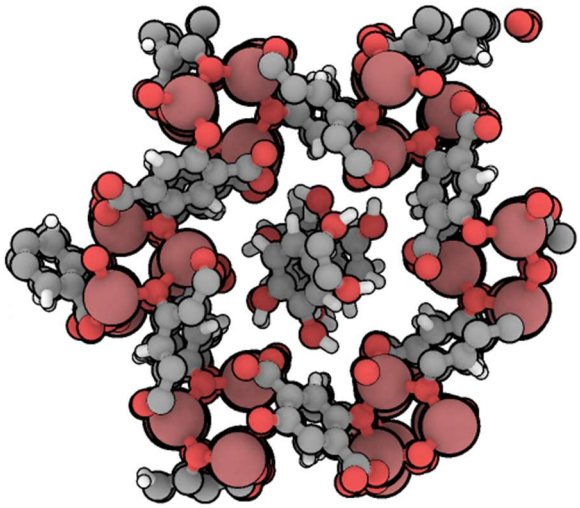

Figure S4. *Snapshot of the configuration of the framework with five molecules of catechol in the same pore (the same for resorcinol)*.

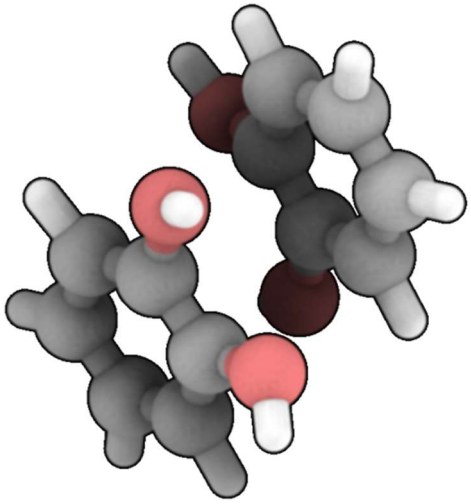

Figure S5. *Snapshot of the π-stacking present for the molecules of catechol corresponding to the initial configuration N=5 (all the molecules in the same pore, c=1).*

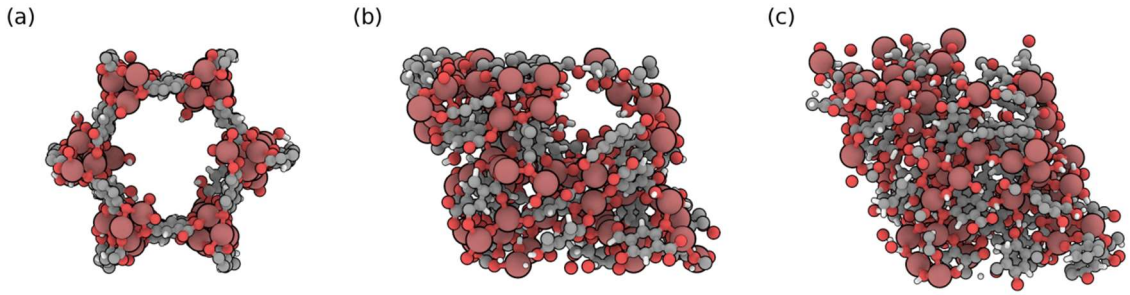

Figure S6. *Snapshot of the configuration of Zn-MOF-74 with (a) a lower content, (b) 10.4 % and (c) a higher content of water. We have reproduced the water instability of Zn-MOF-74 using a ReaxFF. We selected three points to study the behavior of Zn-MOF-74 against water: (i) 10.4 % of water, the amount that causes the structural collapse, (ii) a lower content and (iii) a higher content of water. We obtained the same results described in previous works.*[37,38] *We reproduced the volume change until the 10.4 % of water, when the structural collapse happened.*