

Supporting Information

Guest-modulation of the mechanical behavior of flexible porous Metal Organic Frameworks

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1. Flexible force field parameter for water molecule

Water molecule was described by the TIP4P-2005 model as reported by Abascal and Vega.¹ In this four-site model, a single LJ term is centered only on the oxygen nucleus and electrostatic charges at the hydrogens while the negative charge is placed in a site M along the bisector of the H–O–H angle at 0.1546 Å from the oxygen and coplanar with the oxygen and hydrogens. The H–O bond length and the H–O–H bond angle are fixed at 0.9572 Å and 104.52° respectively. The LJ cross interaction parameters including adsorbate/adsorbate and adsorbate/MOF were determined by the Lorentz-Berthelot mixing rule except for the interaction between the oxygen atoms of the water molecule and the o_c of the MIL-53(Cr) framework where the LJ parameters have been adjusted by our own to describe the stability of the MIL-53(Cr) NP structure loaded with high concentration of water accurately. The corresponding atomic partial charges and potential parameters are given in Table S1.

Table S1 Atomic partial charges and non-bonded potential parameters used for water. The LJ parameters for the water/o_c interactions are also reported.

<i>Atomic partial charges</i>		
Angle type	<i>q (e)</i>	
H_H ₂ O	0.5564	
M_H ₂ O	-1.1128	
<i>Lennard Jones potential</i>		
Atom type	σ_{ii} (Å)	ϵ_{ii} (kJ·mol ⁻¹)
O_H ₂ O	3.15890	0.775474
o_H ₂ O – o_c	3.13945	0.762708

2. Unit cell parameters of the framework

Table S2 Simulated unit cell parameters for the different forms of MIL-53(Cr) under the external applied pressure (P1 symmetry). The α and γ angles for all the structures listed in this table are 90.00°.

P (MPa)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
MIL-53(Cr) ^a					
0.1	17.368	12.562	6.684	90.00	1458
53.5	19.273	7.914	6.583	95.00	1000
300	19.324	7.397	6.556	96.23	931
MIL-53(Cr) loaded with 1 H ₂ O/u.c. ^b					
0.1	17.594	12.205	6.672	90.00	1433
21	19.229	8.107	6.580	94.85	1022
300	19.274	7.622	6.546	96.10	956
MIL-53(Cr) loaded with 4 H ₂ O/u.c. ^b					
0.1	19.169	8.259	6.541	95.50	1031
MIL-53(Cr) loaded with 1 CH ₃ OH/u.c. ^b					
0.1	17.858	11.751	6.665	90.00	1399
7	18.929	9.420	6.636	90.23	1183
300	19.227	7.965	6.543	95.18	998
MIL-53(Cr) loaded with 3 CH ₃ OH/u.c. ^b					
0.1	18.976	9.279	6.618	90.31	1165
MIL-53(Cr) loaded with 0.5 n-hexane/u.c. ^b					
0.1	17.737	11.961	6.672	90.00	1415
10	17.940	11.602	6.666	90.00	1387
300	19.147	8.347	6.548	94.29	1044
MIL-53(Cr) loaded with 1 n-hexane /u.c. ^b					
0.1	18.391	10.727	6.653	90.00	1312

^a Our previous work.²

^b This work.

References

- 1 J. Abascal, C. Vega, *J. Chem. Phys.*, **2005**, *123*, 234505.
- 2 Q. Ma, Q. Yang, A. Ghoufi, G. Férey, C. Zhong, G. Maurin, *Dalton Trans.*, **2012**, *41*, 3915.