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Supporting Information

Impact of mechanical deformation on guest diffusion in zeolitic imidazolate frameworks

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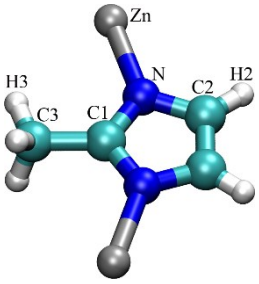
Table S1. Force Field Parameters for ZIF-8 Flexible Framework.[s1]



bond potential: $E_{bond}= K_b(b-b_0)^2$		
bond type	K_b (kcal·mol^{-1}·Å^{-2})	b_0 (Å)
C1-C3	346.543	1.490
C1-N	488.000	1.335
C2-N	440.210	1.370
C2-H2	367.000	1.080
C2-C2	540.249	1.350
C3-H3	340.000	1.090
Zn-N	78.500	2.011

bending potential: $E_{bend}= K_\theta(\theta-\theta_0)^2$		
angle type	K_θ (kcal·mol^{-1}·rad^{-2})	θ_0 (°)
N-C1-N	75.484	112.16
N-C1-C3	66.015	123.92
C2-C2-N	73.750	108.65
C2-C2-H2	49.451	125.67
N-C2-H2	49.954	125.68
C1-C3-H3	48.088	109.32
C1-N-C2	71.254	105.27
C1-N-Zn	48.680	128.33
C2-N-Zn	32.477	126.40
N-Zn-N	35.240	109.48
H3-C3-H3	35.000	109.50

dihedral: $E_{proper}= K_\varphi$ [1+ cos(n φ - φ_0)]			
type[a]	K_φ (kcal·mol^{-1})	n	φ_0 (°)
X-N-C2-X	2.325	2	180.0
X-C2-C2-X	5.150	2	180.0
X-C1-N-X	5.000	2	180.0

improper: $E_{improper}= K_\varphi$ (φ - φ_0)^2		
type[b]	K_φ (kcal·mol^{-1} ·rad^{-2})	φ_0 (°)
N-C3-C1-N	2.000	180.0
C2-H2-C2-N	2.000	180.0
C2-Zn-N-C1	2.000	180.0

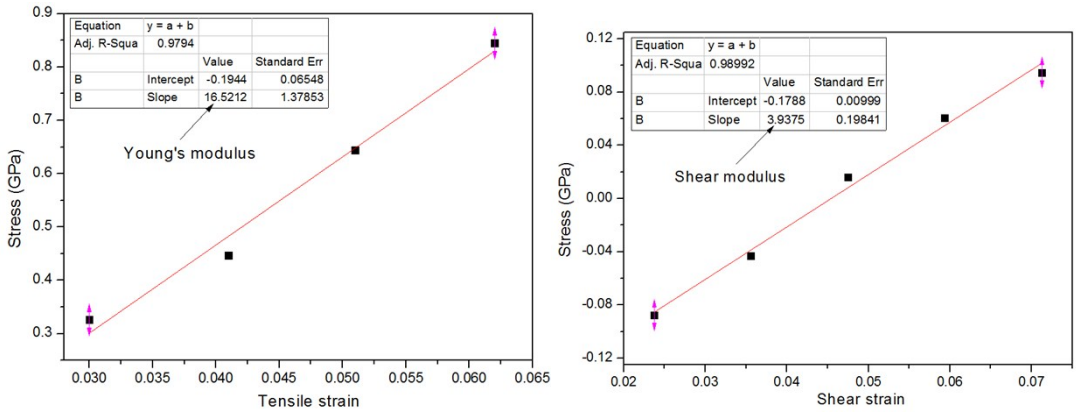
	VDW interaction		partial charges
atom	ε (kcal/mol)	σ (Å)	q (e)
Zn	0.0125	1.960	+0.7362
N	0.1700	3.250	-0.3008
C1	0.0860	3.400	+0.4339
C2	0.0860	3.400	-0.1924
C3	0.1094	3.400	-0.6024
H2	0.0150	2.511	+0.1585
H3	0.0157	2.650	+0.1572

[a] X denotes wildcard atoms: the given potential term is repeated for each possible dihedral combination X-A-B-X having A-B as central atoms.

[b] Improper term A-B-C-D refers to the angle between planes A-B-C and B-C-D, with B-C axis of rotation.

Table S2. Force Field Parameters for CO_2 Molecules[s2] and H_2 Molecules[s3].

non-bonded interaction			
atom type	ε (kcal/mol)	σ (Å)	q (e)
C	0.05584	2.757	+ 0.6512
O	0.15982	3.033	– 0.3256
H	0.00147	3.314	0.0000



(a) (b)

Figure S1. Linear fitting the stress-strain data to obtain (a) the Young's modulus and (b) the shear modulus of ZIF-8.

H2ZIF8.indata: including the initial configuration of H2ZIF8 system and all related force field parameters.
CO2ZIF8.indata: including the initial configuration of CO2ZIF8 system and all related force field parameters.

CO2ZIF8(NVE)-unstrained.inrun: using CO2ZIF8.indata as input to perform NVE equilibrium the system. It will output the file "0.restart.50000000".
CO2ZIF8(NVE)-tenisle.inrun: using "0.restart.50000000" as starting point to perform uniaxial tensile deformation of ZIF-8. At every strain point, the system will be performed NVE equilibrium for 50 ns to collect data for guest diffusion computation.
CO2ZIF8(NVE)-shear.inrun: using "0.restart.50000000" as starting point to perform shear deformation of ZIF-8. At every strain point, the system will be performed NVE equilibrium for 50 ns to collect data for guest diffusion computation.

CO2ZIF8(NPT)-unstrained.inrun: using CO2ZIF8.indata as input to perform NPT equilibrium the system. It will output the file "0.restart.50000000". It should be noted that the different commands were used for later tensile and shear deformation (marked inside this file).
CO2ZIF8(NPT)-tenisle.inrun: using "0.restart.50000000" as starting point to perform uniaxial tensile deformation of ZIF-8. At every strain point, the system will be performed NPT equilibrium for 50 ns to collect data for guest diffusion computation.
CO2ZIF8(NPT)-shear.inrun: using "0.restart.50000000" as starting point to perform shear deformation of ZIF-8. At every strain point, the system will be performed NPT equilibrium for 50 ns to collect data for guest diffusion computation.

Regarding to H2ZIF8 system, you only have to replace the character of "CO2" with the "H2" in above files with suffix "inrun".

Calculate the self-diffusion rate by mean squared displacement using the Einstein relation:

$$D_S = \frac{1}{2d_0} \lim_{t\to\infty} \frac{d}{dt} \left\langle \frac{1}{N} \sum_{i=1}^{N} \left[\mathbf{r}_i(t) - \mathbf{r}_i(t_0)\right]^2 \right\rangle$$

where d_0 is the dimensionality of the system and $\mathrm{r}_i(t)$ is the position vector of the sorbate molecule i at time t. The D_S value is averaged over all the N sorbed molecules and over multiple time origins t_0 (as symbolized by the brackets).

References

s1. B. Zheng, M. Sant, P. Demontis, G. B. Suffritti, *J. Phys. Chem. C*, 2012, **116**, 933.
s2. J. G. Harris, K. H. Yung, *J. Phys. Chem.*, 1995, **99**, 12021.
s3. F. Grazzi, M. Santoro, M. Moraldi, L. Ulivi, *Phys. Rev. B*, 2002, **66**, 144303.