Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Molecular simulation of gas adsorption and diffusion in a breathing MOF using a rigid force field

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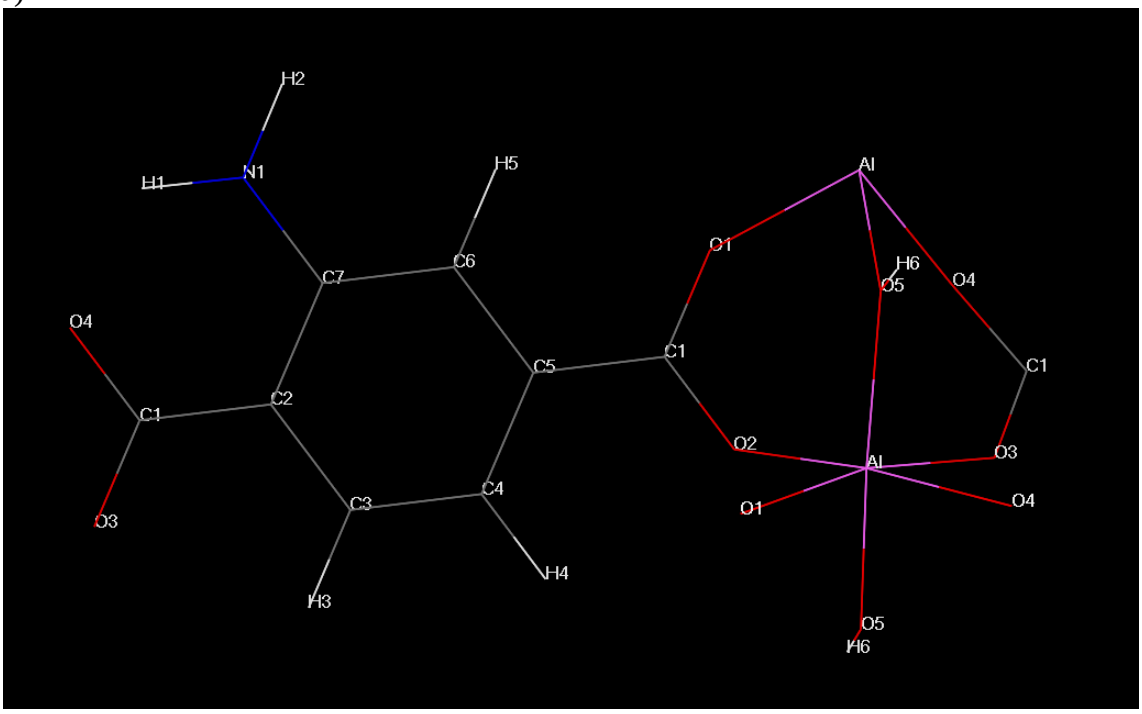
Figure 1. Crystallographic positions of the different atoms for the (a) *np* form and (b) *lp* form of NH_2-MIL-53(Al). The other labels follow by symmetry.

a)



b)

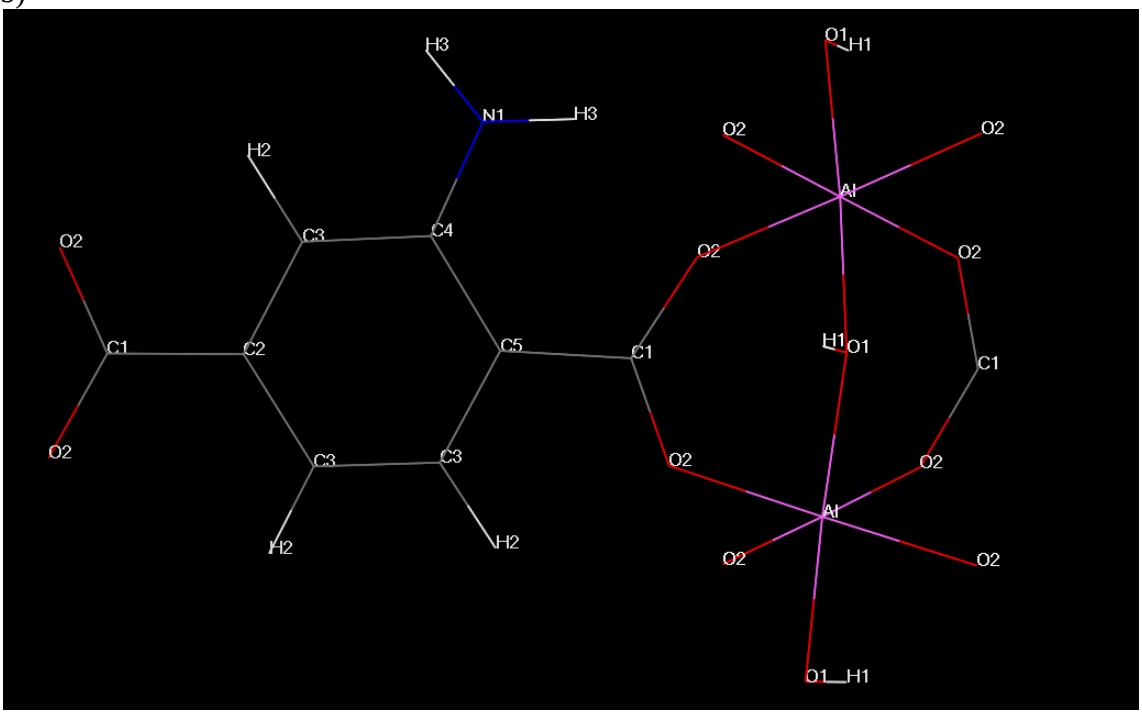
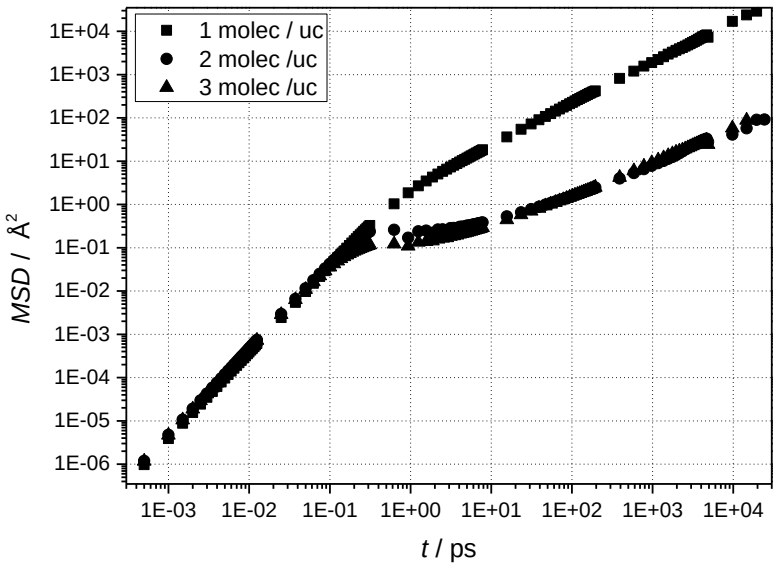


Figure 2. Mean Square Displacement (MSD) as a function of the time for different number of molecules of carbon dioxide in NH_2-MIL-53(Al) for a) *np* form and b) *lp* form at 273 K.

a)



b)

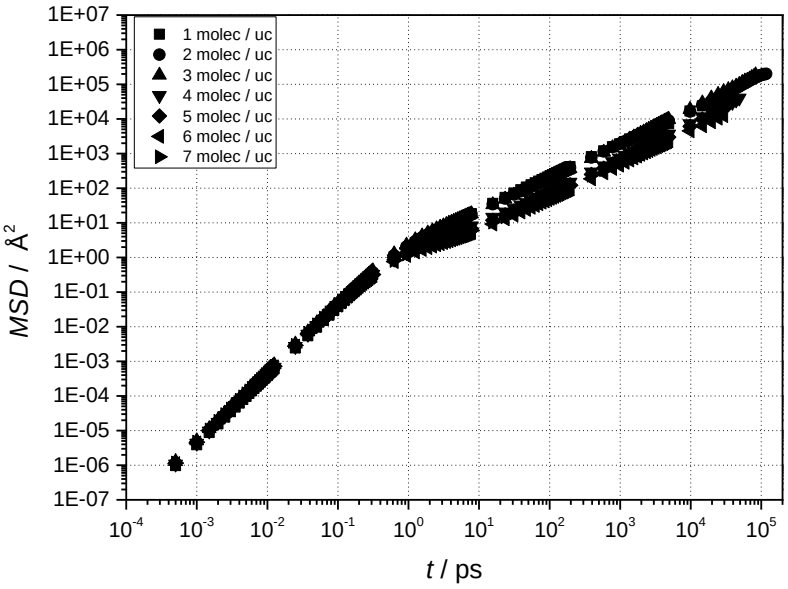


Table I. Crystallographical information for the (a) *np* form and (b) *lp* form of NH_2-MIL-53(Al).

a)

19.7839	7.8496	6.5934	90.0000	73.5673	90.0000			
Al	0.000000000	0.000000000	0.000000000	**Al**	Al	1.422
N1	2.739527715	5.378781428	-1.501715397	**N1**	N	-0.554
O2	7.715366747	4.664232342	-2.038376667	**O1**	O	-0.517
O3	8.593682425	5.232543165	-0.159809433	**O2**	O	-0.533
O5	2.333063882	6.761645365	2.305315859	**O3**	O	-0.556
O4	1.454587732	6.193334074	0.426875231	**O4**	O	-0.626
O1	1.420121801	6.983788941	4.640607843	**O5**	O	-0.710
C2	2.456975673	6.340121619	1.144405015	**C1**	C	0.569
C1	7.591294175	5.085755620	-0.877339264	**C1**	C	0.573
C4	3.740640402	6.026216060	0.638921521	**C2**	C	-0.097
C6	4.882929822	6.193255939	1.456498186	**C3**	C	-0.125
C5	6.166415254	5.879742925	0.951077971	**C4**	C	-0.136
C3	6.307790402	5.399190032	-0.371982235	**C5**	C	-0.070
C7	5.165519042	5.232229223	-1.189495667	**C6**	C	-0.149
C8	3.881817443	5.545742237	-0.684138685	**C7**	C	0.205
H2	10.718433186	5.990579139	-4.336925621	**H1**	H	0.306
H3	4.688908051	4.842732293	3.854082490	**H2**	H	0.265
H6	4.769043762	6.580554803	2.522611100	**H3**	H	0.167
H5	7.087017241	6.014363443	1.609983528	**H4**	H	0.133
H4	5.279386720	4.845008493	-2.255671908	**H5**	H	0.143
H1	9.461984366	2.108245443	-1.67784086	**H6**	H	0.290

b)

17.4426	12.0429	6.8447	90.0000	89.9900	90.0000			
Al1	4.402861231	3.018311944	3.466239959	**Al**	Al	1.480
Al2	13.121370776	9.069989441	6.805785302	**Al**	Al	1.480
N1	9.758960702	6.840969717	6.047284762	**N1**	N	-0.458
N2	16.520060824	11.208567626	2.618791339	**N1**	N	-0.458
O1	4.312508541	2.197949736	1.751900872	**O1**	O	-0.720
O2	13.028051936	9.888064159	8.514685013	**O1**	O	-0.720
O3	3.022279334	1.804869355	4.115834802	**O2**	O	-0.580
O4	11.948181031	7.638088609	7.433650018	**O2**	O	-0.580
O5	14.431483739	10.265007032	3.898454194	**O2**	O	-0.580
O6	5.895424124	4.025580217	7.421231258	**O2**	O	-0.580
O7	14.277291768	10.497314218	6.148895797	**O2**	O	-0.580
O8	5.796001440	4.205260241	2.836634049	**O2**	O	-0.580
O9	2.750349250	2.081856080	6.350855577	**O2**	O	-0.580
O10	11.665610806	7.810663722	2.834852446	**O2**	O	-0.580
C1	2.377426335	1.656260037	5.205261862	**C1**	C	0.560
C2	11.327224357	7.376637506	8.526092928	**C1**	C	0.560
C3	14.843303452	10.723479798	5.027216717	**C1**	C	0.560
C4	6.353292456	4.403245568	1.706466018	**C1**	C	0.560
C5	1.070801236	0.927905457	5.147675208	**C2**	C	-0.060
C6	7.659743218	5.132081801	8.535788357	**C2**	C	-0.060
C7	0.659853538	0.358155850	3.951765715	**C3**	C	-0.083
C8	8.123542291	5.670519988	7.342358663	**C3**	C	-0.083
C9	16.491280956	12.184162770	6.197811435	**C3**	C	-0.083
C10	8.441520735	5.238059321	2.858519712	**C3**	C	-0.083

C11	0.241056732	0.840353563	6.285666858	**C3**	C	-0.083
C12	9.642443929	5.926190544	2.798427663	**C3**	C	-0.083
C13	9.352198935	6.365756839	7.259958029	**C4**	C	0.210
C14	16.878854759	11.700038964	3.836799738	**C4**	C	0.210
C15	10.111649754	6.525686245	8.459007763	**C5**	C	-0.110
C16	16.070041924	11.558052724	5.008129121	**C5**	C	-0.110
H1	3.827952916	1.359402549	1.761535696	**H1**	H	0.296
H2	12.541926685	10.725768185	8.512615756	**H1**	H	0.296
H3	1.294589800	0.461724772	3.074180620	**H2**	H	0.127
H4	7.529272648	5.542503820	6.440054968	**H2**	H	0.127
H5	15.838927590	12.099501059	7.063483210	**H2**	H	0.127
H6	8.104529509	4.769109001	3.779552365	**H2**	H	0.127
H7	0.537755350	1.331222207	7.209137432	**H2**	H	0.127
H8	10.262179003	-427.525709435	3.686635545	**H2**	H	0.127
H9	10.623589763	7.375192549	6.005888250	**H3**	H	0.215
H10	15.673920037	10.647730451	2.558341730	**H3**	H	0.215
H11	9.068058824	6.983797951	5.320736128	**H3**	H	0.215
H12	17.212706212	11.151604875	1.882422526	**H3**	H	0.215

Table II. Charge parameters for the adsorbed molecules used in this work.

Adsorbed Molecules	**Charge [e^-]**
O_co_2	**0.652**
C_co_2	**-0.326**
CH_4	**-**

Table III. Lennard-Jones interaction parameters for NH_2-MIL-53(Al) and adsorbed molecules used in this work.

Atom	ε/κ_B [K]	σ [Å]
NH_2-MIL-53(Al)		
Al	**156.0**	**3.91**
O	**48.19**	**3.03**
C	**47.86**	**3.74**
H	**7.65**	**2.85**
N	**38.95**	**3.26**
Adsorbed Molecules		
O_co_2	**85.67**	**3.02**
C_co_2	**29.93**	**2.74**
CH_4	**158.50**	**3.72**

Lorentz-Berthelot mixing rules were used to calculate mixed Lennard-Jones parameters. Except for the O_co_2 – $H_{\_OH}$ interaction for the *np* structure NH_2-MIL-53(Al):

$\varepsilon_{O\_co_2\text{-}H\_OH}/\kappa_B$ = 25.60 K and $\sigma_{O\_co_2\text{-}H\_OH}$ = 2.58 Å