Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information:

Molecular dynamics simulations probe greenhouse gas sorption capabilities of metal organic framework-based membrane for efficient gas separation processes

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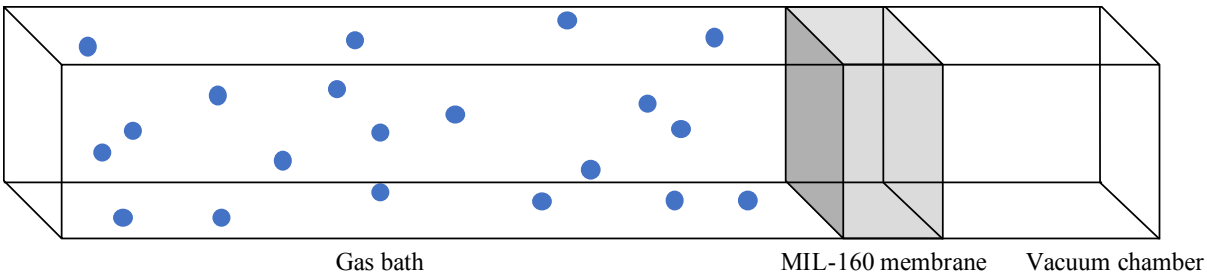

Figure S.1: schematic representation of gas permeation simulations at initial configurations in which a 4 x 4 x 3 MIL-160 membrane separates a gas bath from a vacuum chamber.

Tables:

Table S.1: varied simulation pressures corresponded to respective number of molecules in single-component gas baths as well as simulation box dimensions required to achieve target pressure calculated for ideal gas conditions.

Simulation pressure (bar)	Number of molecules	X-direction length (nm)	Y-direction length (nm)	Z-direction length (nm)	Simulation box volume (nm^3)
0.2	20	8.4	8.4	68.1	4,805
0.5	50	8.4	8.4	68.1	4,805
1	100	8.4	8.4	68.1	4,805
5	500	8.4	8.4	68.1	4,805
50	500	8.4	8.4	15.1	1,065

Table S.2: varied simulation pressures corresponded to respective number of molecules in gas mixture baths as well as simulation box dimensions required to achieve target pressure calculated for ideal gas conditions.

Simulation pressure (bar)	Number of CO_2 molecules	Number of balance molecules	X-direction length (nm)	Y-direction length(nm)	Z-direction length (nm)	Simulation box volume (nm^3)
0.2	1	19	8.4	8.4	68.1	4,805
0.5	2	48	8.4	8.4	68.1	4,805
1	5	95	8.4	8.4	68.1	4,805
5	25	475	8.4	8.4	68.1	4,805
50	25	475	8.4	8.4	15.1	1,065

Figures and Figure captions:

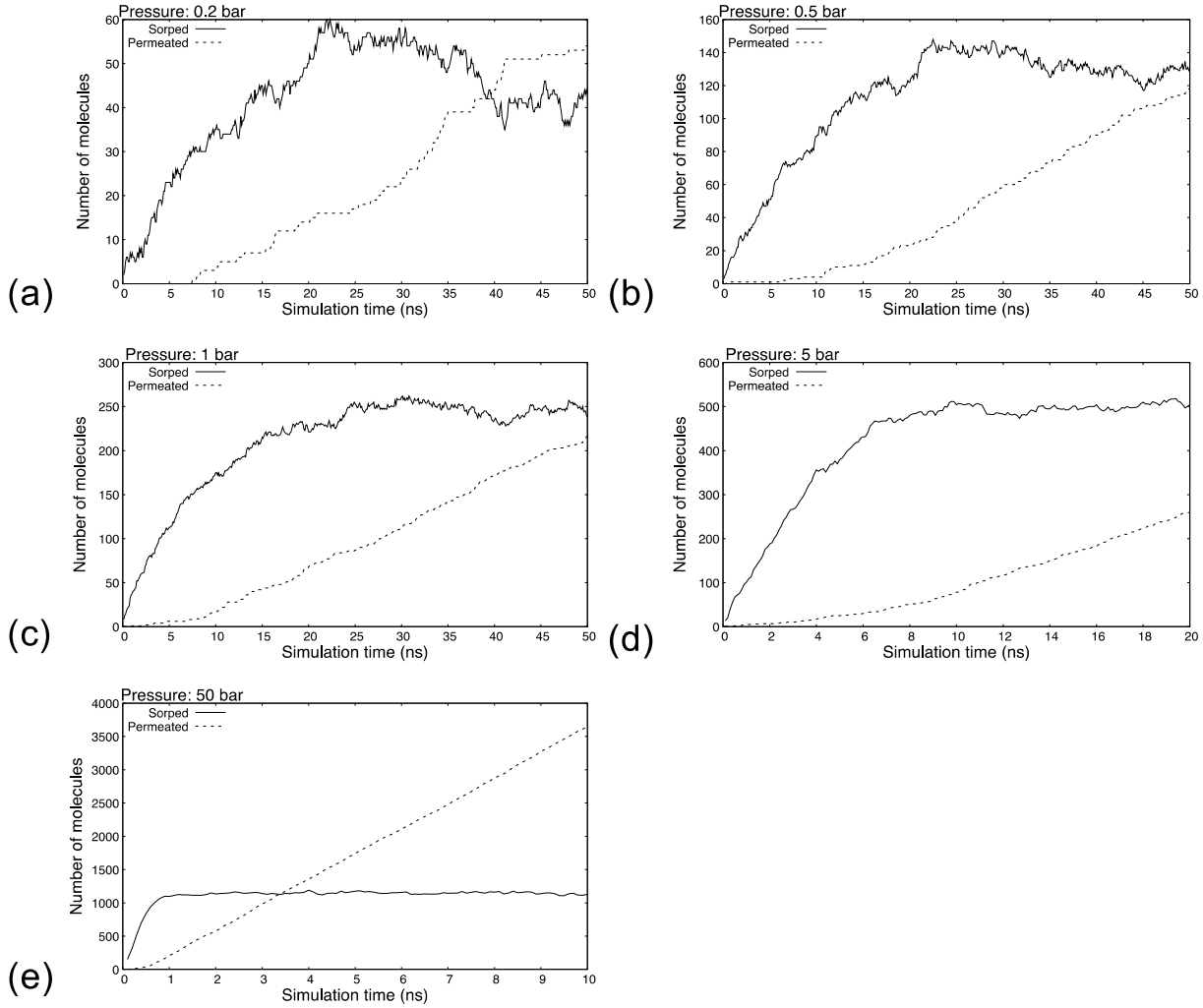

Figure S.2: permeation and sorption profiles of CO_2 at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, (d) 5 bar, and (e) 50 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.

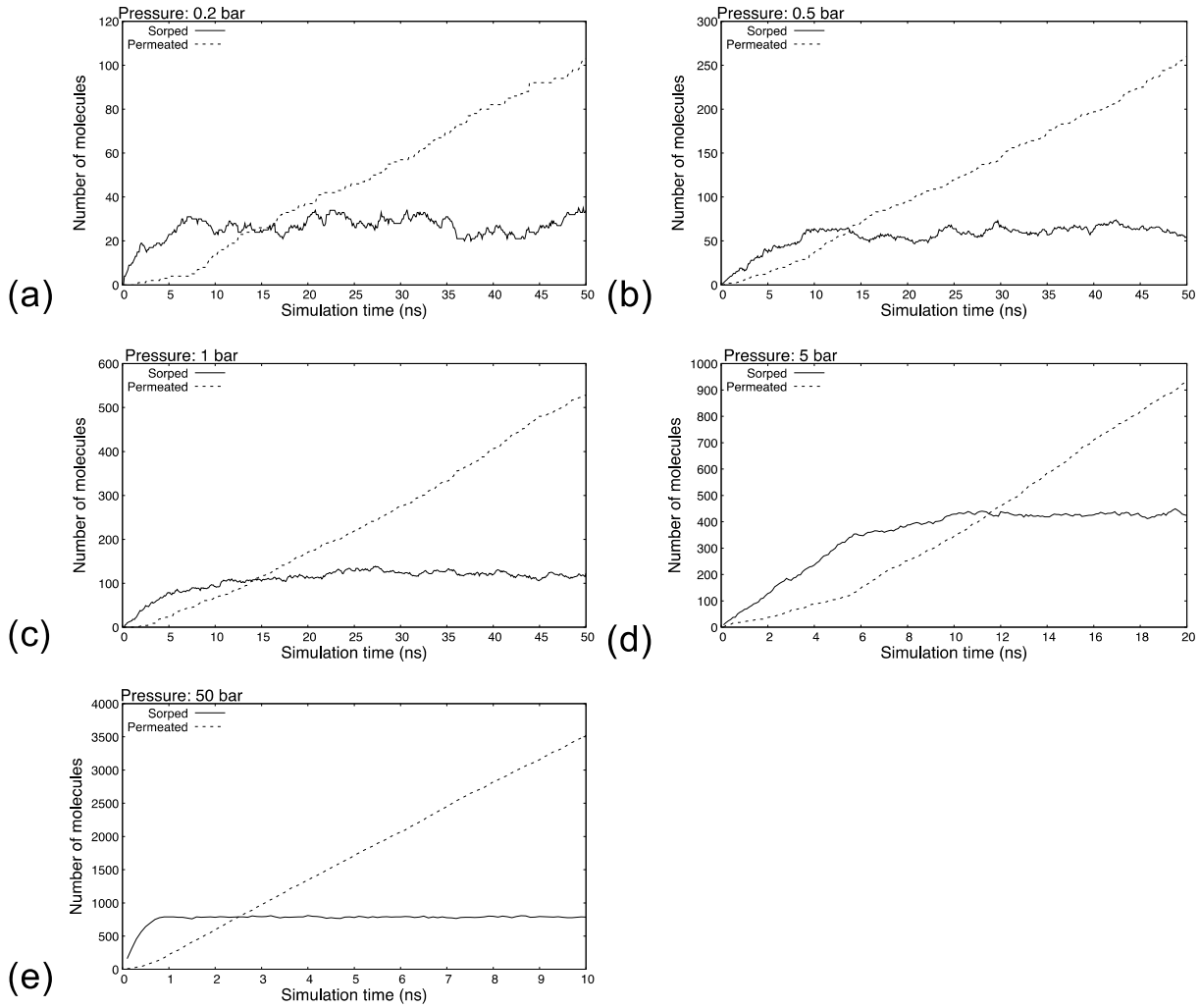

Figure S.3: permeation and sorption profiles of CH_4 at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, (d) 5 bar, and (e) 50 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.

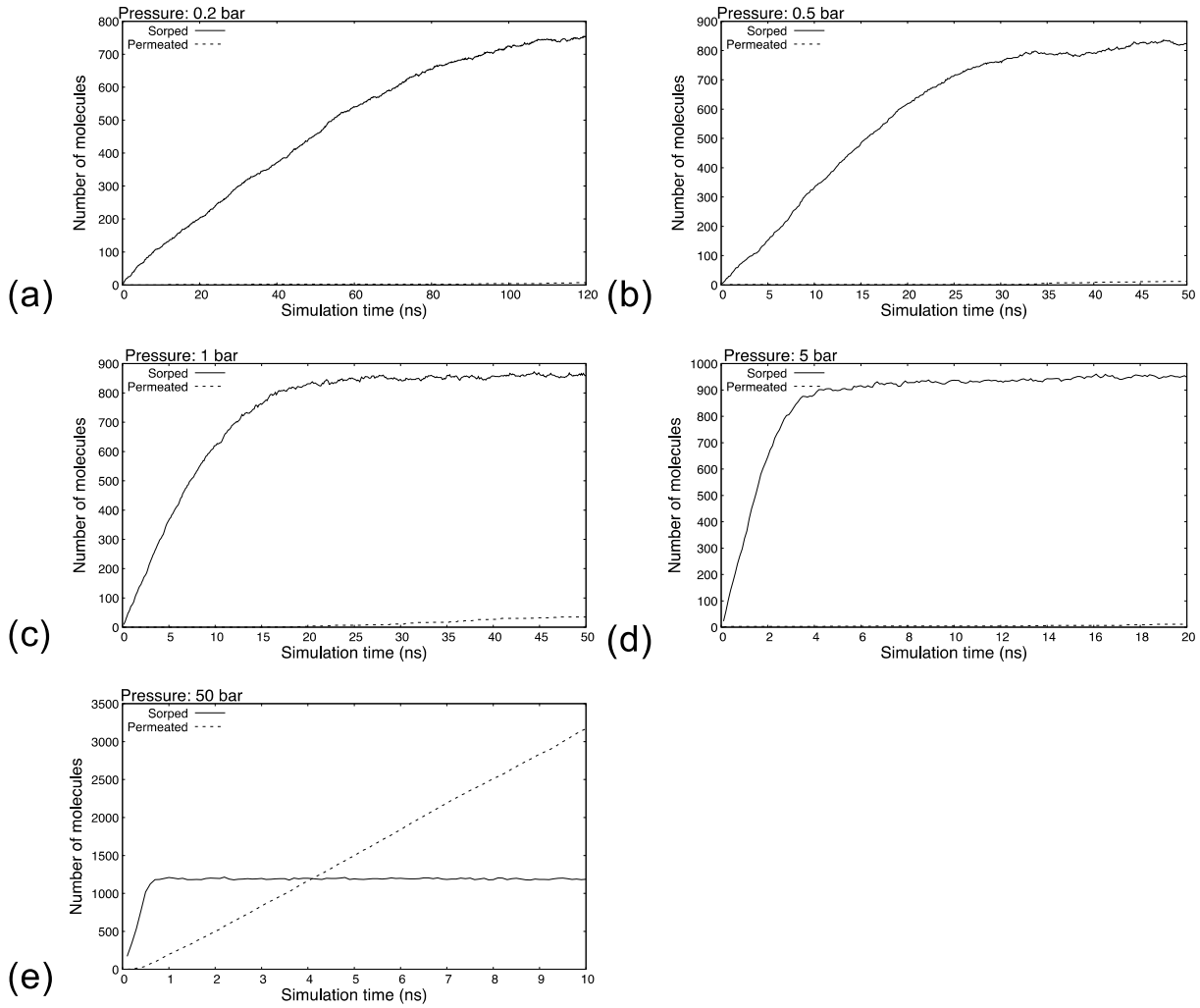

Figure S.4: permeation and sorption profiles of SO_2 at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, (d) 5 bar, and (e) 50 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.

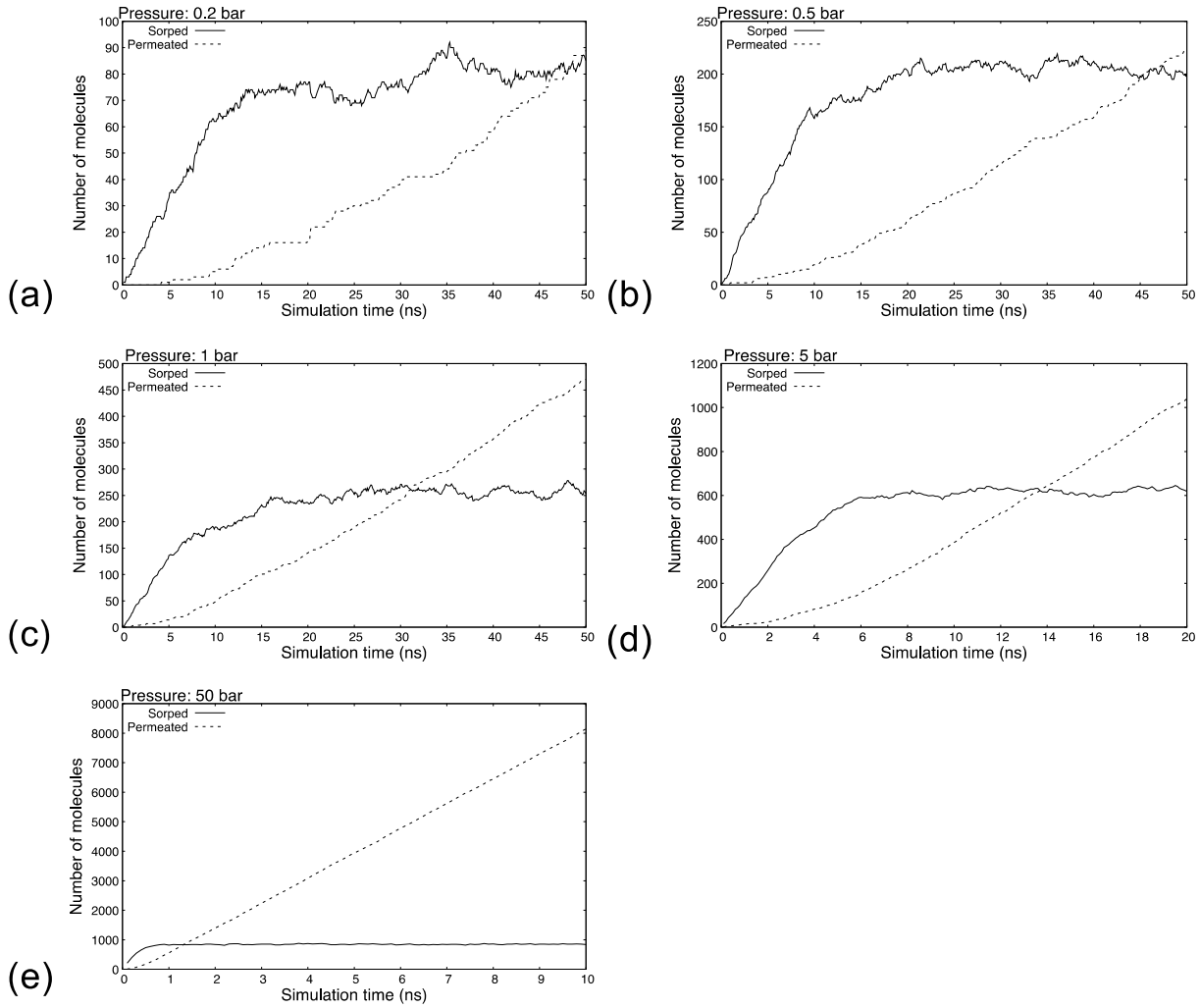

Figure S.5: permeation and sorption profiles of NO_2 at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, (d) 5 bar, and (e) 50 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.

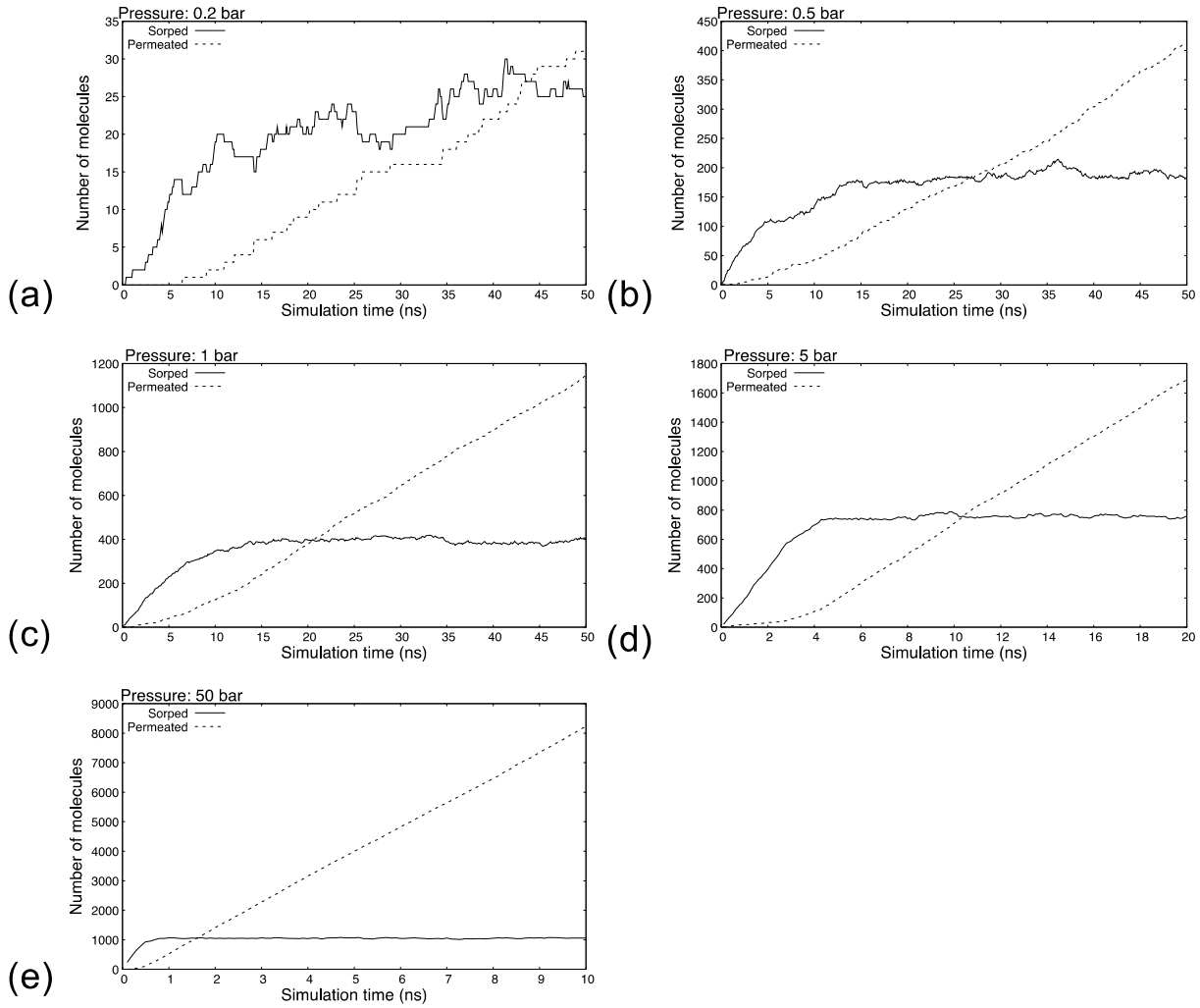

Figure S.6: permeation and sorption profiles of NO at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, (d) 5 bar, and (e) 50 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.

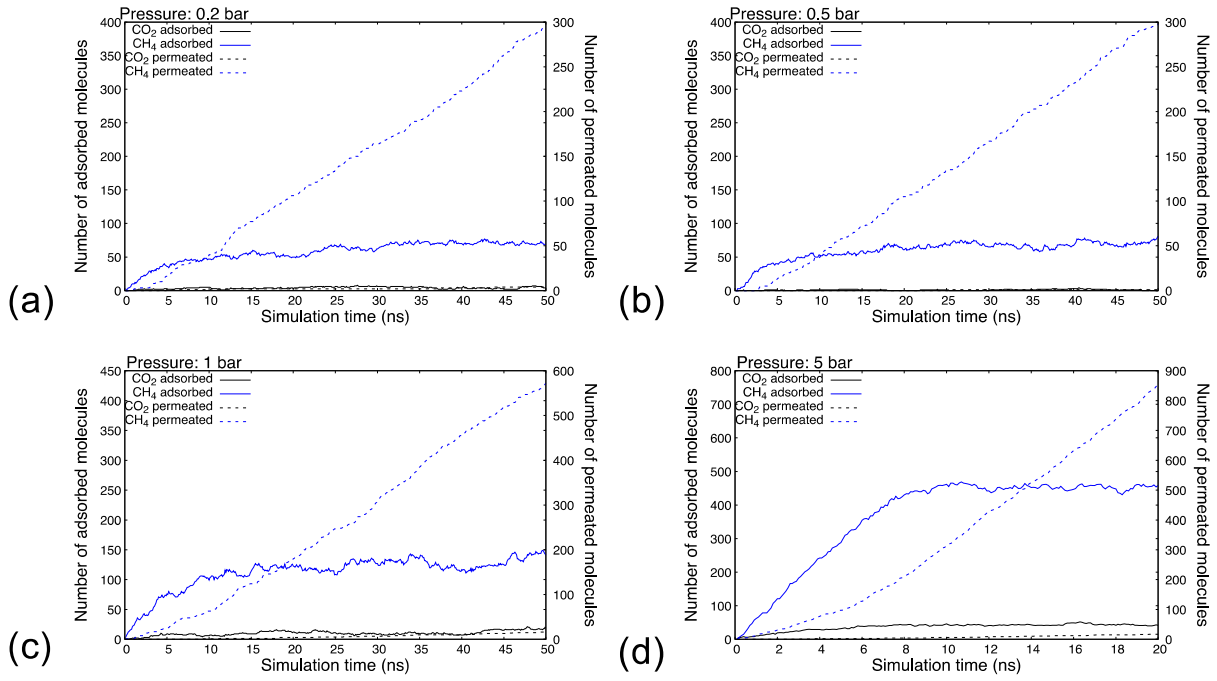

Figure S.7: permeation (dashed line) and sorption (solid line) profiles of CO_2 (black) and CH_4 (blue) at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, and (d) 5 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.

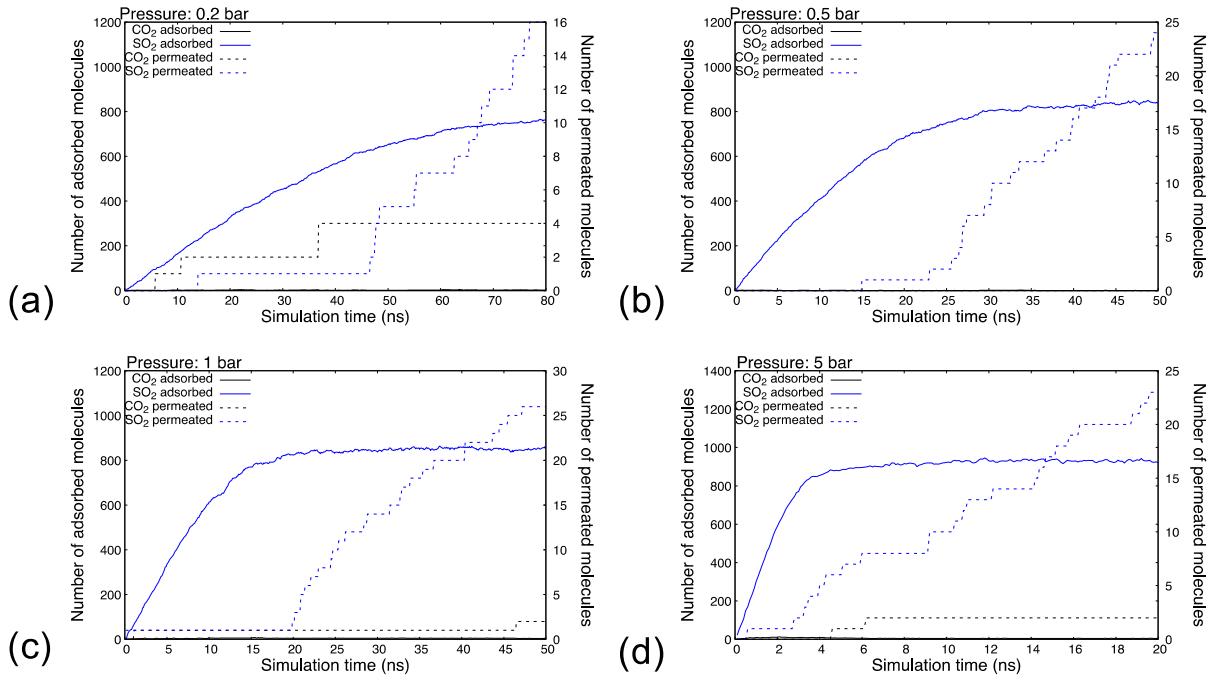

Figure S.8: permeation (dashed line) and sorption (solid line) profiles of CO_2 (black) and SO_2 (blue) at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, and (d) 5 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.

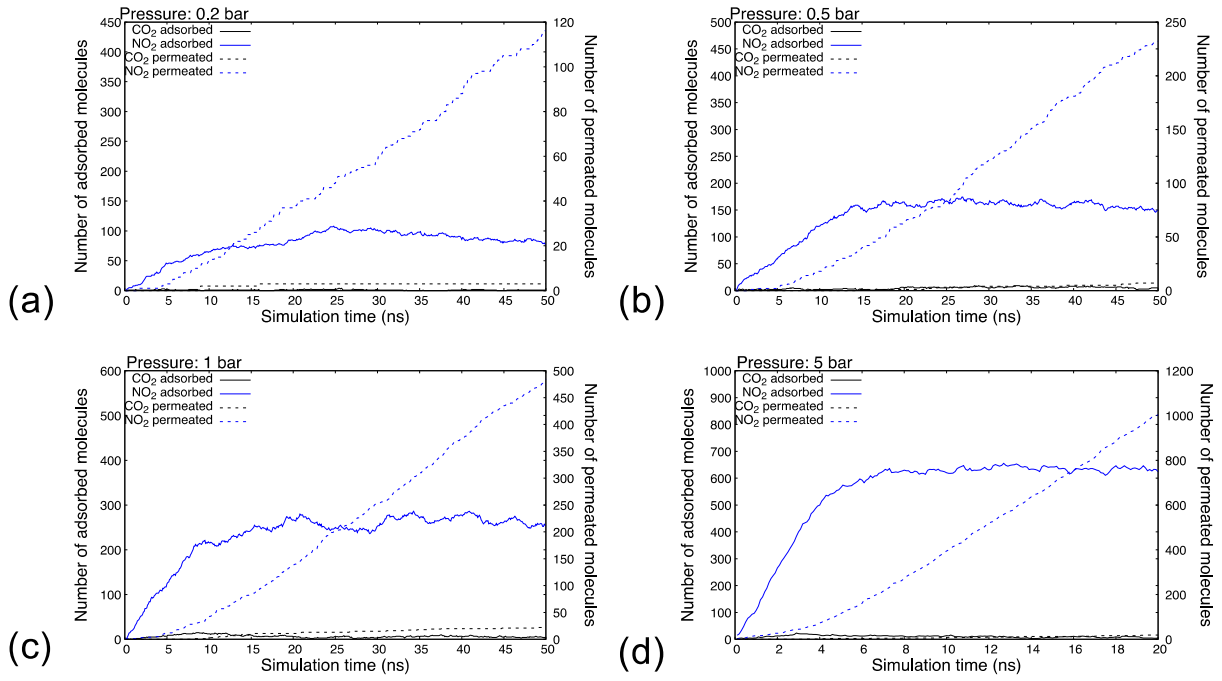

Figure S.9: permeation (dashed line) and sorption (solid line) profiles of CO_2 (black) and NO_2 (blue) at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, and (d) 5 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.

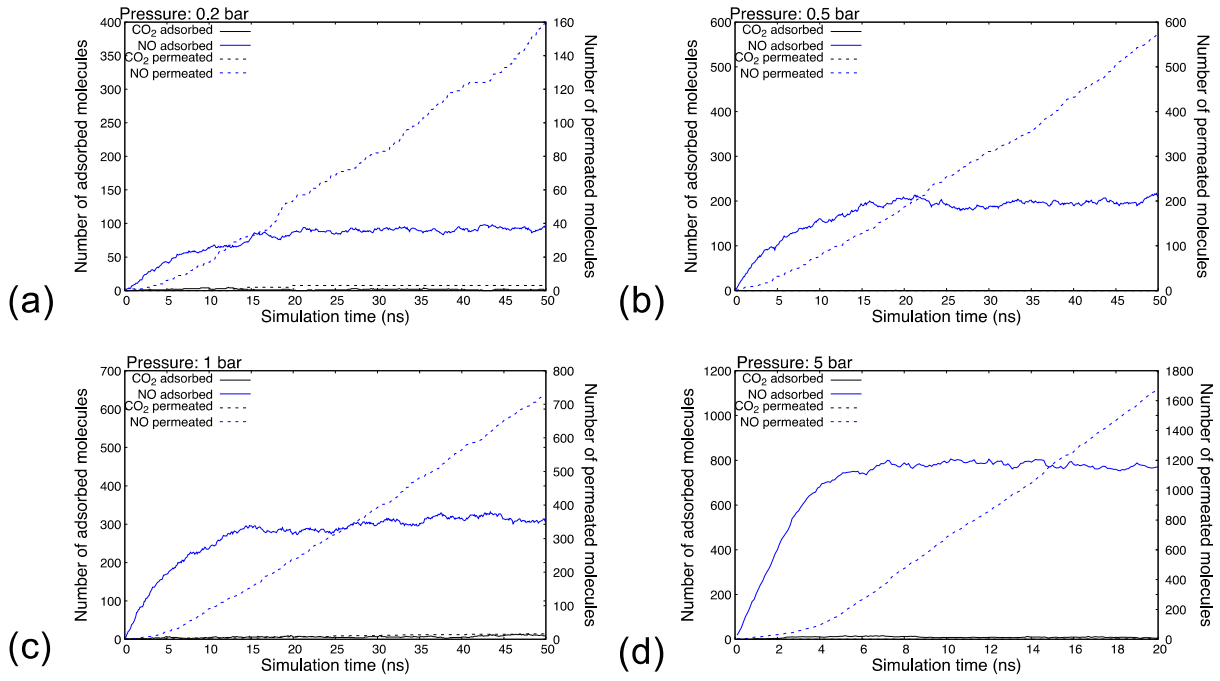

Figure S.10: permeation (dashed line) and sorption (solid line) profiles of CO_2 (black) and NO (blue) at (a) 0.2 bar, (b) 0.5 bar, (c) 1 bar, and (d) 5 bar with respect to a rigid 4 x 4 x 3 MIL-160 membrane.