Supplementary Information for

Selective Gas Diffusion in Graphene Oxides Membranes: A Molecular Dynamics Simulations Study

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This material includes supplementary tables, figures and their captions.

Table S1. (a) The atomic van der Waals radii and (b) van der Waals sizes of the gas molecules (along the long axis if the molecule is not spherical).

(a)

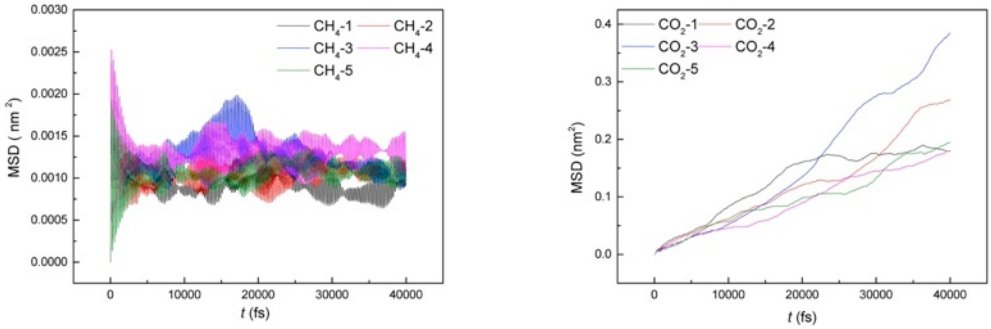
Atom	He	C	O	N	H
van der Waals radius (nm)	0.14	0.17	0.152	0.155	0.12

(b)

Molecule	He	H_2	N_2	O_2	CO	CH_4	CO_2
Size (nm)	0.28	0.314	0.42	0.425	0.436	0.456	0.536

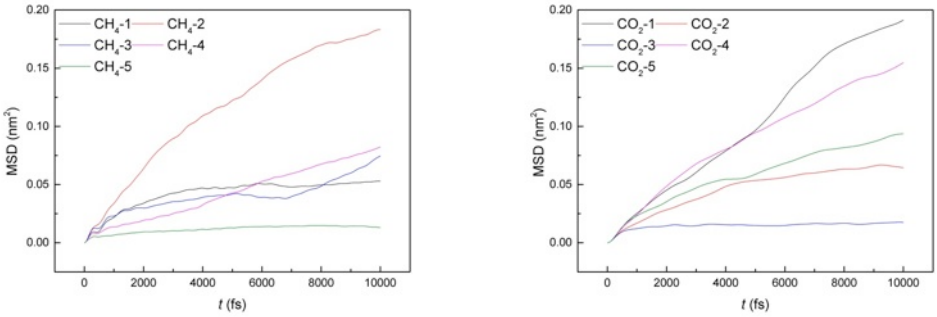
Table S2. Diffusion coefficients for gases between GO sheets with an interlayer distance d = 1 nm, which are functionalized by hydroxyl and epoxy groups respectively.

D (mm^2/s)	He	CH_4	CO_2	N_2
hydroxyl	0.391	0.133	0.030	0.086
expoxy	1.027	0.333	0.091	0.134



(a) (b)

Figure S1. The mean-square displacements of (a) CH_4 and (b) CO_2 molecules diffusing between graphene sheets with d = 0.55 nm. The five curves plotted represent five different positions randomly chosen as the initial configurations of MD simulations.



(a) (b)

Figure S2. The mean-square displacements of (a) CH_4 and (b) CO_2 molecules diffusing between graphene sheets with d = 0.6 nm. The five curves plotted represent five different positions randomly chosen as the initial configurations of MD simulations.