Supplementary Information for:

Insights into CO_2/N_2 separation through nanoporous graphene from molecular dynamics"

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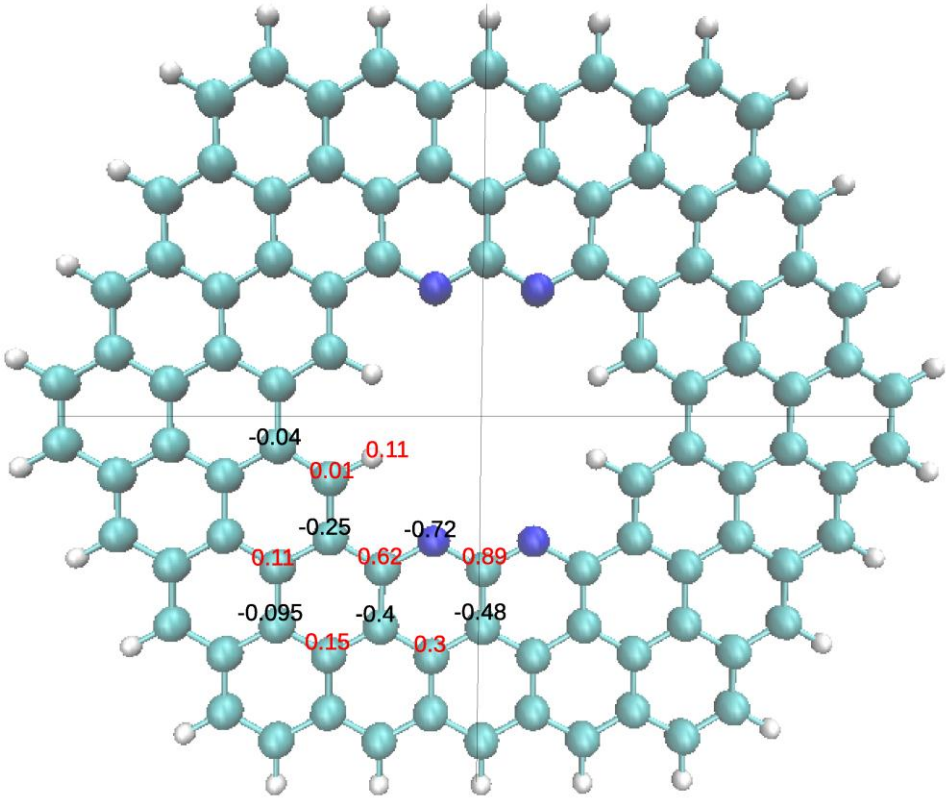

Figure S1. The fragmental cluster of nanoporous graphene (C: cyan, N: blue and H: white). The atomic charges were denoted on each atom (positive in red; negative in black). Due to the symmetry, only the lower left part was listed.

Table S1. Partial charges of rim atoms of 4N4H nanopores: C (black), N (blue), and H (orange). The shaded area denotes the net deletion of 6 C atoms in each 4N4H nanopore.

-0.095	0.15	-0.40	0.30	-0.48	0.30	-0.40	0.15	-0.095
0.11	-0.25	0.62	**-0.72**	0.89	**-0.72**	0.62	-0.25	0.11
-0.04	0.01	0.11				0.11	0.01	-0.04
-0.04	0.01	0.11				0.11	0.01	-0.04
0.11	-0.25	0.62	**-0.72**	0.89	**-0.72**	0.62	-0.25	0.11
-0.095	0.15	-0.40	0.30	-0.48	0.30	-0.40	0.15	-0.095

Table S2. Force field parameters for porous graphene.

Lennard-Jone parameters		
	ε (K)	σ (Å)
C	28	3.4
H	15.1	2.42
N	85.6	3.25
Bonds		
	length (Å)	
C-C	1.42	
C-H	1.10	
N-C	1.42	

Table S3. Force field parameters (van der Waals terms and partial charges) for gas molecules.

CO_2			
	ε (K)	σ (Å)	q (e)
C	28.129	2.757	0.6512
O	80.507	3.033	-0.3256
bonds	length (Å)		
C-O	1.149		
N_2			
	ε (K)	σ (Å)	q (e)
N	36.4	3.318	-0.4048
Center-Of-Mass	0	0	0.8096
bonds	length (Å)		
N-N	1.098		

Table S4. The system size and pressure studied in this work.

CO_2		N_2	
Number	Pressure (atm)	Number	Pressure (atm)
2000	52.5	700	28.4
1500	44.0	500	20.3
1000	32.8	250	10.2
550	19.9	125	5.1
250	9.7		
125	5.0		
70	2.8		