Supporting Information

Porous Germanene As A Highly Efficient Gas Separation Membrane

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Table S1 The calculated energy barriers $\boldsymbol{E}_b$ (eV) for common gases (H_2, H_2O, N_2, CO, CO_2 and CH_4) and noble gases (He, Ne, Ar) penetrating through the 585 porous germanene.

E_b (eV)	585 Germanene	Silicene [1,2]
H_2	0.27	0.34
H_2O	0.27	0.45
N_2	0.72	1.03
CO	1.13	0.99
CO_2	0.49	1.01
CH_4	1.08	1.66
He	0.25	0.57
Ne	0.35	1.18
Ar	0.94	2.89

Table S2 The selectivity (S) of H_2 relative to other common gases (H_2O, N_2, Co, CO_2, CH_4) and He relative to other noble gases (Ne, Ar) for the 585 porous germanene at T = 300 K.

	585 Germanene	Silicene [1,2]	Graphene [3]

	S	S	S
H_2	--	--	--
H_2O	10	10^2	--
N_2	10^7	10^{12}	--
CO	10^7	10^{11}	--
CO_2	10^4	10^{10}	--
CH_4	10^{13}	10^{13}	10^{23},10^8
He	_	_	_
Ne	10	10^3	_
Ar	10^{11}	10^{18}	_

Details of Molecular Dynamic Simulation

In order to show the superiority of our porous germanene during gas permeation, the ab initio molecular dynamic simulations (MD) with a Nose-Hoover thermostat is taken into consideration through VASP package. The constant-volume and constant-temperature (NVT) ensemble were employed during the simulation with a time step of 1 fs. The electrostatic interaction and van der Waals interaction were calculated using the atom based method. In simulation, we added a mixture gas of 31 H_2 and 18 CH_4 molecules, placed between the monolayer pure germanium and 555777 porous germanene with a distance of 6 Å. MD simulation is performed at the room temperature with a time span of 50 ps. From snapshots in Fig. S1, H_2 molecule in mixed gases can permeate through the pore of the 555777 porous germanene to the vacuum layer freely, while the CH_4 molecule is confined between the two layers from beginning to end.

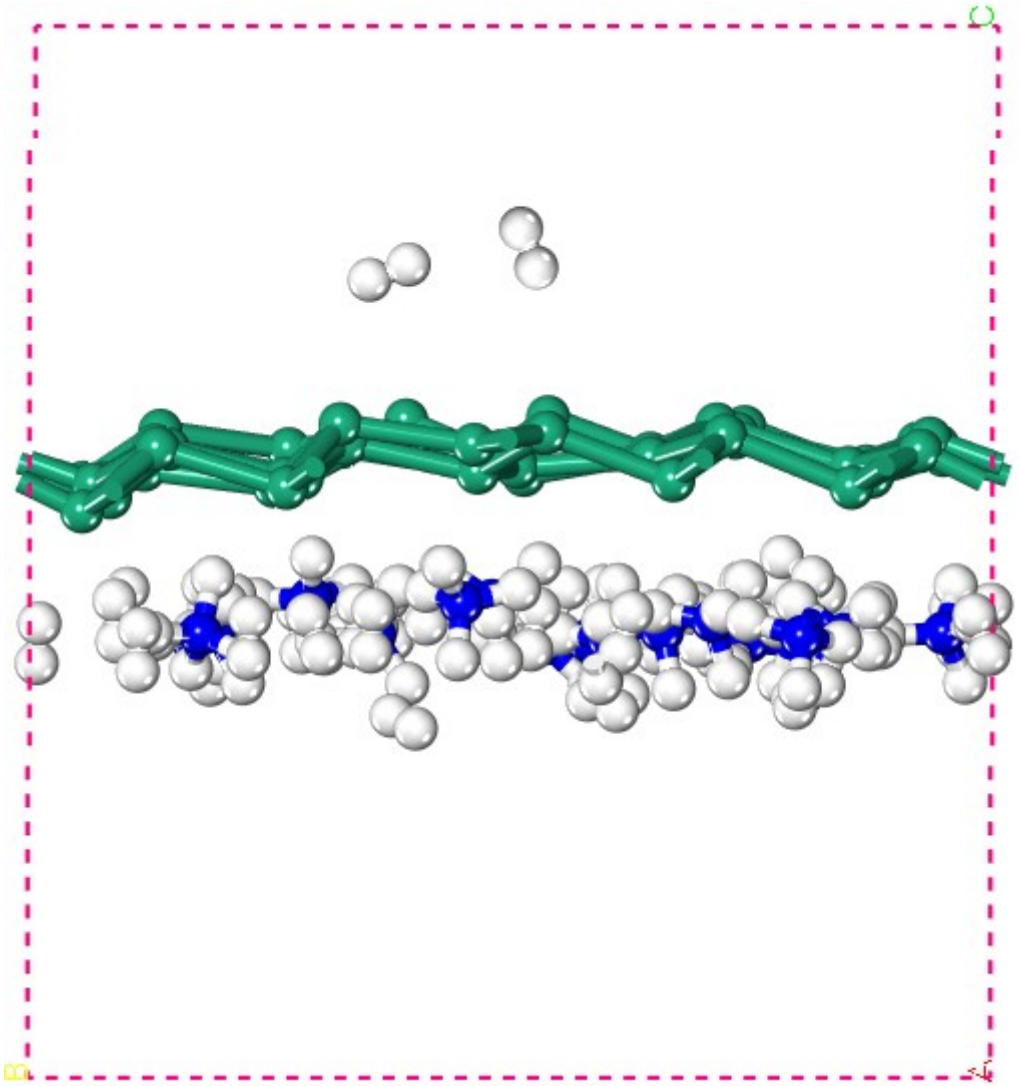

Figure S1. Snapshots of gas mixture permeating through 555777 porous germanene nanosheet in MD simulation in the 0-50 ps at 300 K. The blue, grey, and green beads represent the C, H, and Ge atoms respectively.

References:

(1) W. Hu, X. Wu, Z. Li, and J. Yang, Phys. Chem. Chem. Phys., 2013, 15, 5753-5757.

(2) W. Hu, X. Wu, Z. Li, and J. Yang, Nanoscale, 2013, 5, 9062-9066.

(3) D. E. Jiang, V. R. Cooper, and S. Dai, Nano Lett., 2009, 9, 4019-4024.