

A promising monolayer membrane for oxygen separation from harmful gases: Nitrogen-substituted polyphenylene

Ruifeng Lu,^{*a} Zhaoshun Meng,^a Dewei Rao,^b Yunhui Wang,^a Qi Shi,^a Yadong Zhang,^a Erjun Kan,^{a,c} Chuanyun Xiao^{*a,c} and Kaiming Deng^{*a,c}

^a Department of Applied Physics, Nanjing University of Science and Technology, Nanjing 210094, P.R. China. E-mail: rflu@njust.edu.cn

^b Institute for Advanced Materials, Jiangsu University, Zhenjiang 212013, P.R. China

^c Key Laboratory of Soft Chemistry and Functional Materials, Ministry of Education, Nanjing University of Science and Technology, Nanjing 210094, P.R. China. E-mail: cxiao@njust.edu.cn; kmdeng@njust.edu.cn

Figures S1-S7: Electron densities of the transition-state geometries.

Figures S8-S15: Atomic charges computed from Mulliken population analyses of the transition-state geometries.

Table S1: The initial, transition-state, final configurations, and their total energies for the studied gases passing through PG-based membranes.

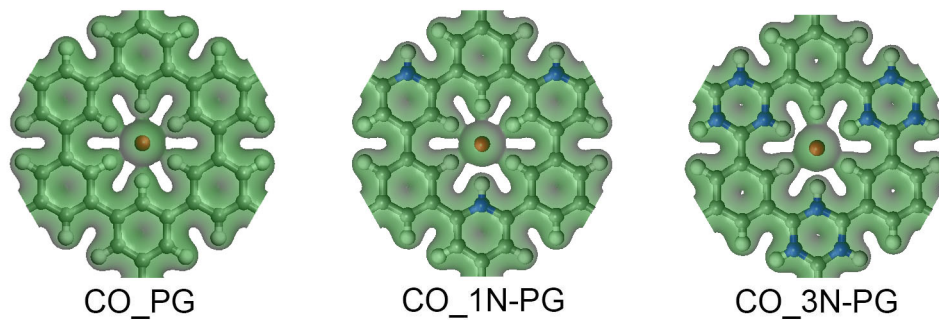


Fig. S1 Electron densities of the transition-state structures for CO passing through PG, 1N-PG and 3N-PG. The isovalue is 0.15 a.u. (C, gray; H, white; N, blue; O, red).

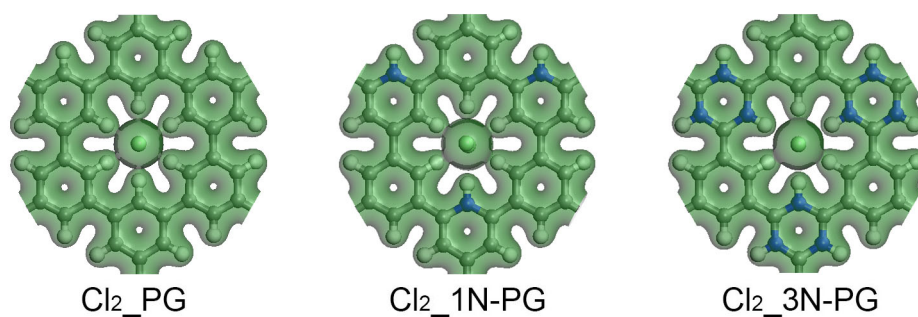


Fig. S2 Electron densities of the transition-state structures for Cl₂ passing through PG, 1N-PG and 3N-PG. The isovalue is 0.20 a.u. (C, gray; H, white; N, blue; O, red; Cl: light green).

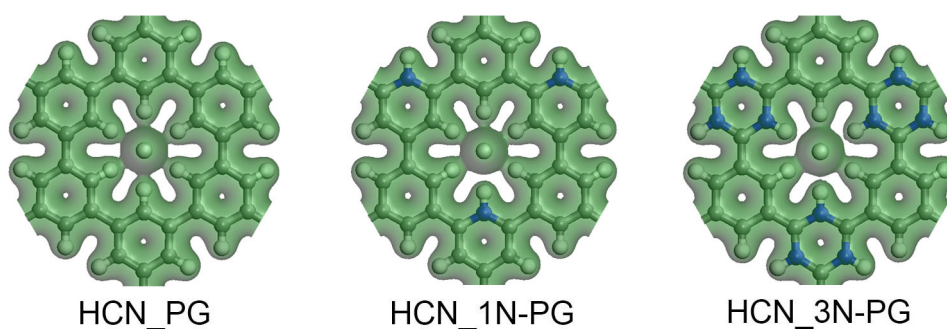


Fig. S3 Electron densities of the transition-state structures for HCN passing through PG, 1N-PG and 3N-PG. The isovalue is 0.19 a.u. (C, gray; H, white; N, blue; O, red).

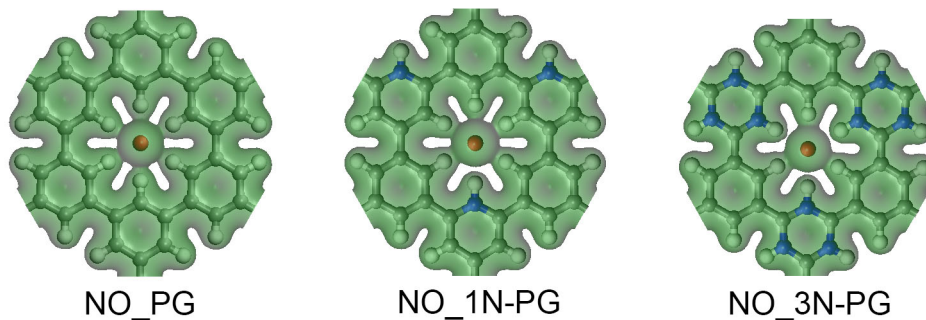


Fig. S4 Electron densities of the transition-state structures for NO passing through PG, 1N-PG and 3N-PG. The isovalue is 0.15 a.u. (C, gray; H, white; N, blue; O, red).

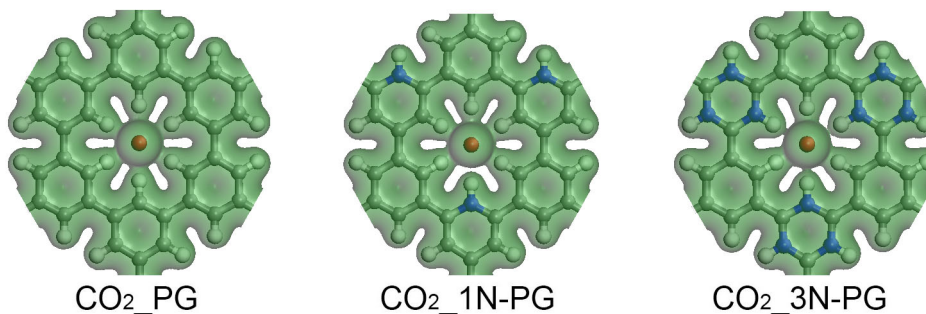


Fig. S5 Electron densities of the transition-state structures for CO₂ passing through PG, 1N-PG and 3N-PG. The isovalue is 0.15 a.u. (C, gray; H, white; N, blue; O, red).

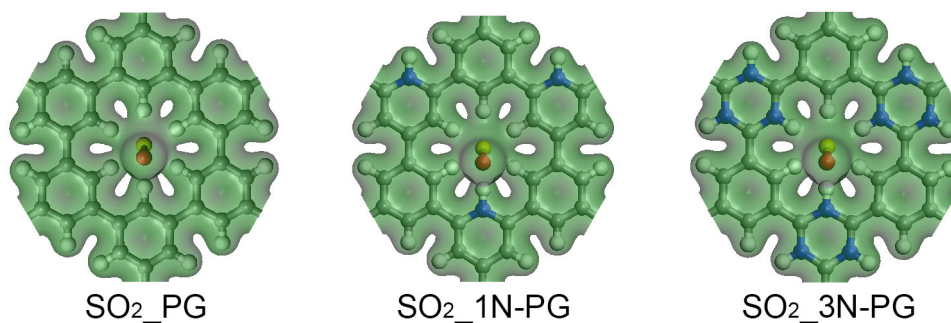


Fig. S6 Electron densities of the transition-state structures for SO₂ passing through PG, 1N-PG and 3N-PG. The isovalue is 0.15 a.u. (C, gray; H, white; N, blue; O, red; S, yellow).

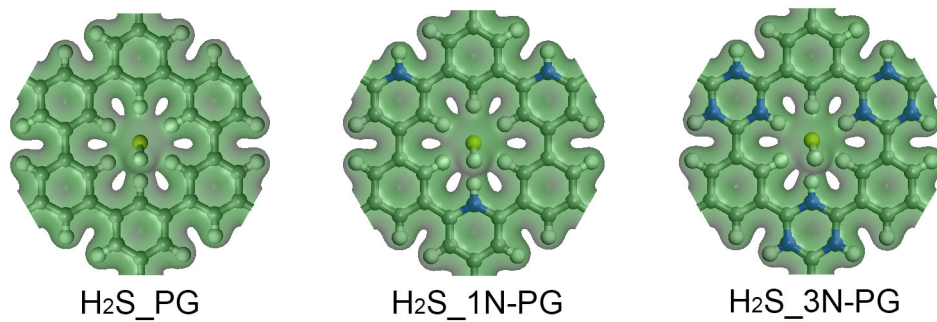


Fig. S7 Electron densities of the transition-state structures for H₂S passing through PG, 1N-PG and 3N-PG. The isovalue is 0.15 a.u. (C, gray; H, white; N, blue; O, red; S, yellow).

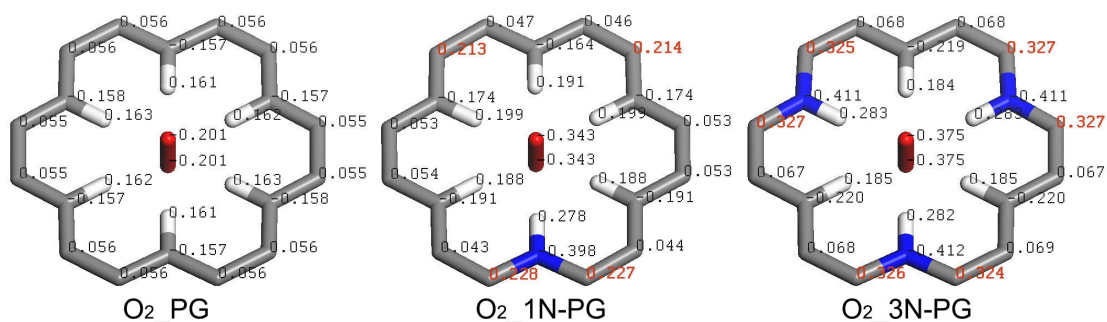


Fig. S8 Atomic charges computed from Mulliken population analyses of the transition-state structures for O₂ passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red.)

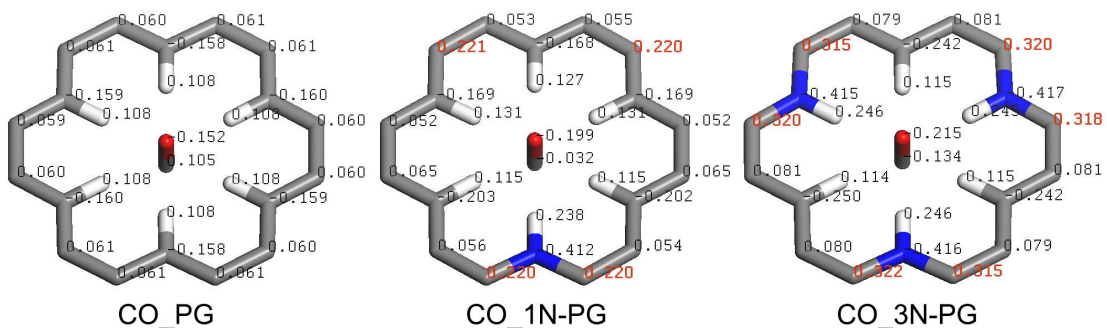


Fig. S9 Atomic charges computed from Mulliken population analyses of the transition-state structures for CO passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red.)

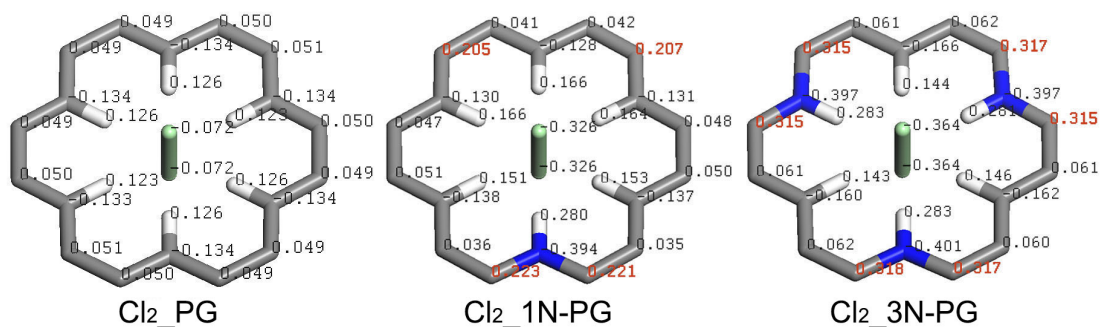


Fig. S10 Atomic charges computed from Mulliken population analyses of the transition-state structures for Cl₂ passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red; Cl, light green.)

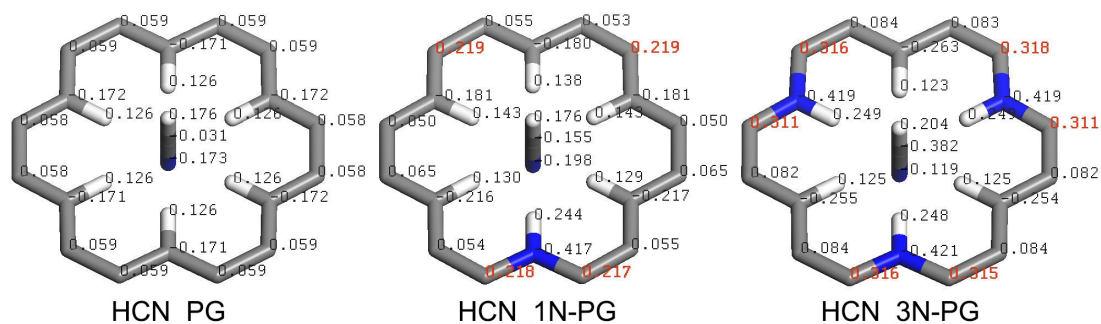


Fig. S11 Atomic charges computed from Mulliken population analyses of the transition-state structures for HCN passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red.)

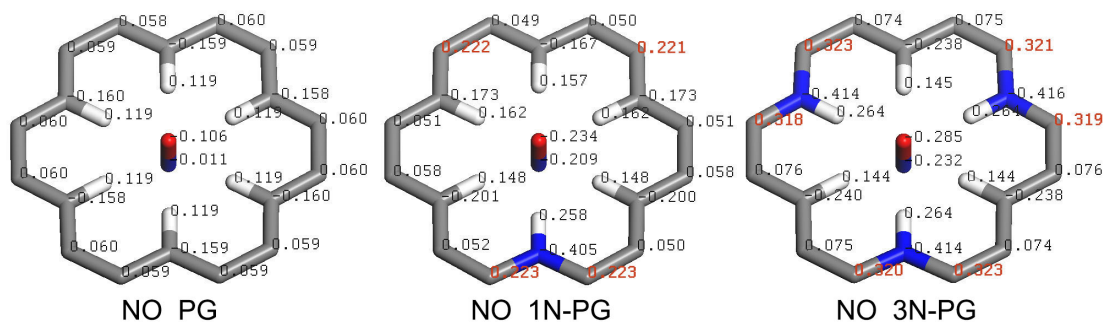


Fig. S12 Atomic charges computed from Mulliken population analyses of the transition-state structures for NO passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red.)

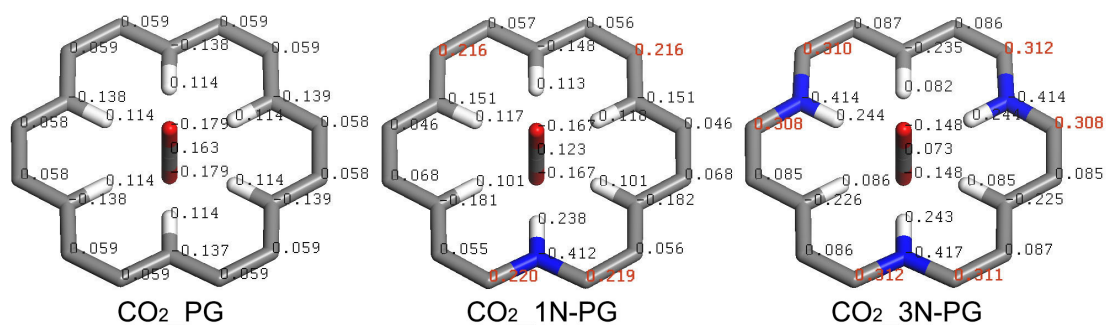


Fig. S13 Atomic charges computed from Mulliken population analyses of the transition-state structures for CO₂ passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red.)

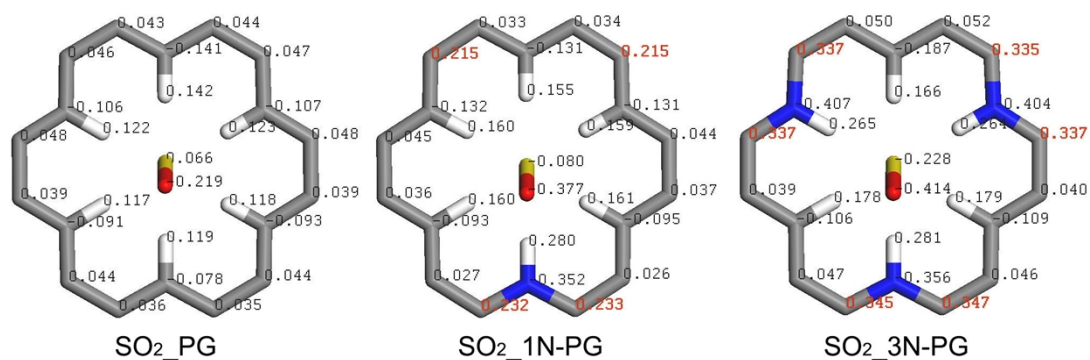


Fig. S14 Atomic charges computed from Mulliken population analyses of the transition-state structures for SO₂ passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red; S, yellow.)

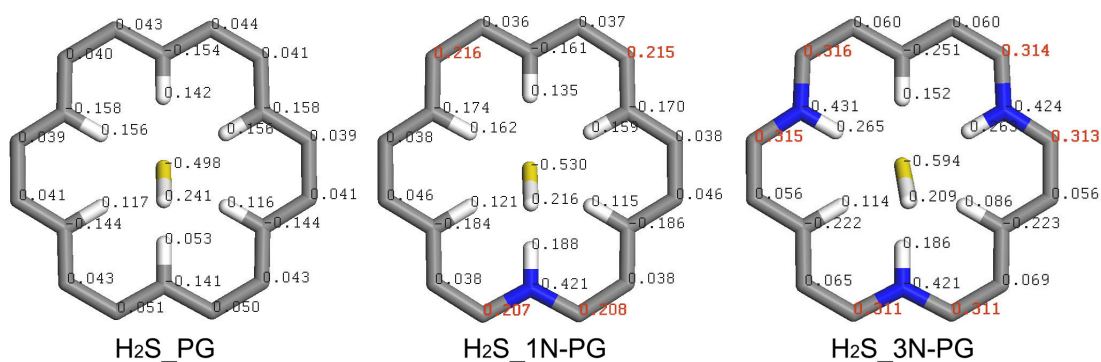


Fig. S15 Atomic charges computed from Mulliken population analyses of the transition-state structures for H₂S passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red; S, yellow.)

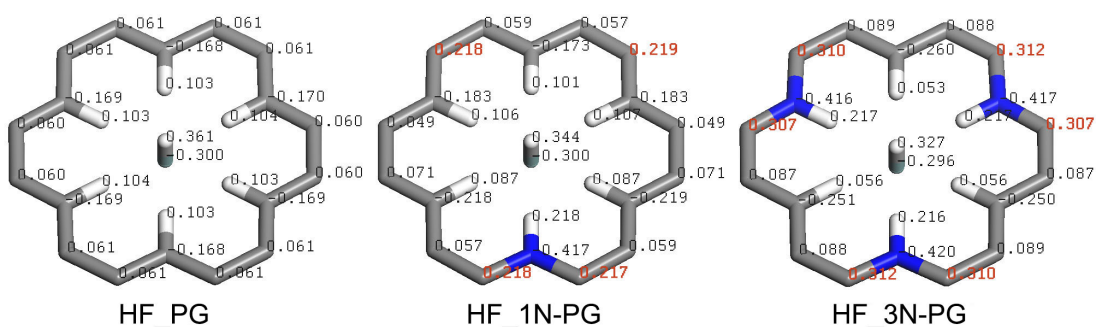


Fig. S16 Atomic charges computed from Mulliken population analyses of the transition-state structures for HF passing through PG, 1N-PG and 3N-PG. (Only the atoms around the pores are drawn for clarity: C, gray; H, white; N, blue; O, red; F, light blue.)

Table S1 The initial, transition-state, and final configurations for the studied gases passing through PG, and their total energies are in Hartree. (C, gray; H, white; N, blue; O, red; Cl, light green; S, blue; F, light blue.)

Gas	Property	Initial State	Transition State	Final State
O ₂	Top view			
	Side view			
	Total energy	-1992.2389698	-1992.1978962	-1992.2389698
CO	Top view			
	Side view			
	Total energy	-1955.2642203	-1955.1787357	-1955.2608557
Cl ₂	Top view			
	Side view			
	Total energy	-2762.0788987	-2761.9895108	-2762.0788987
HCN	Top view			
	Side view			
	Total energy	-1935.3811051	-1935.2938272	-1935.3690994
NO	Top view			
	Side view			
	Total energy	-1971.8339982	-1971.7650242	-1971.8309752
CO ₂	Top view			

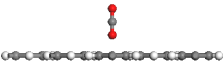
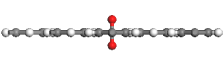
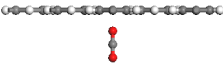
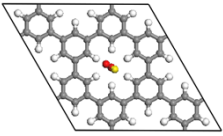
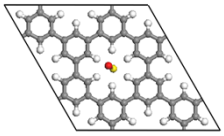
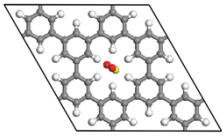
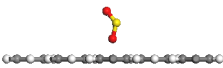
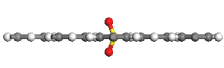
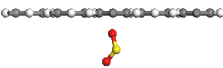
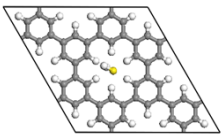
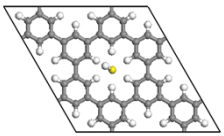
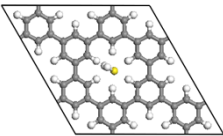
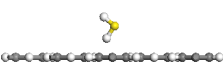
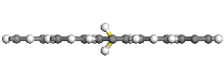
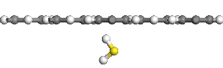
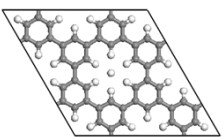
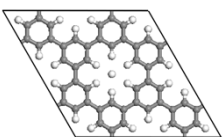
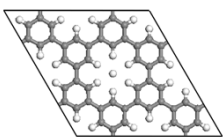
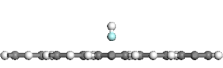
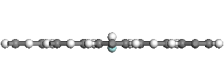
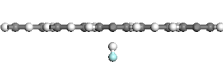
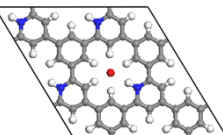
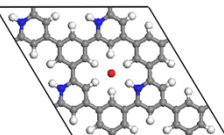
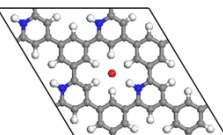
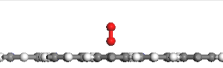
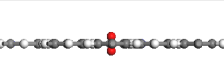
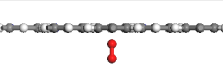
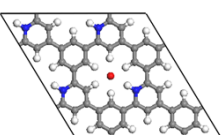
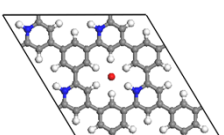
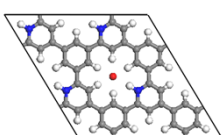
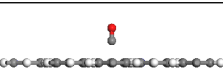
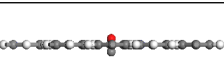
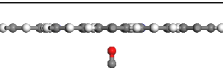
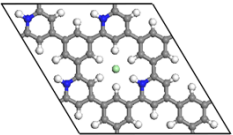
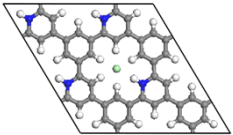
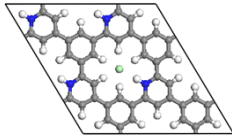
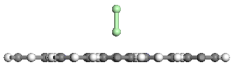
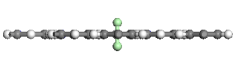
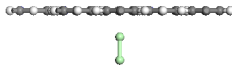
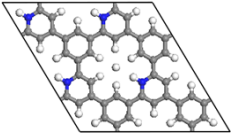
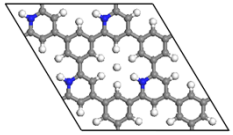
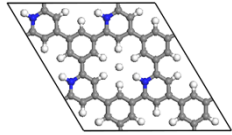
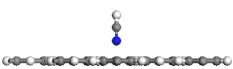
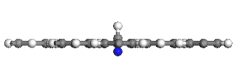
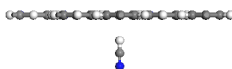
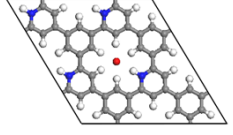
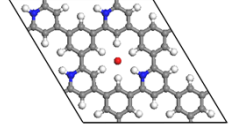
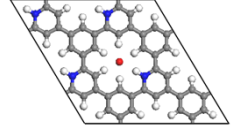
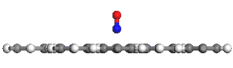
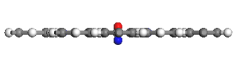
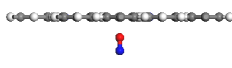
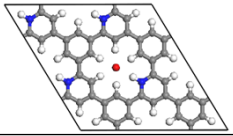
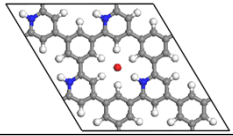
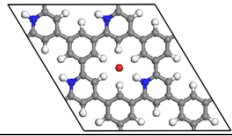

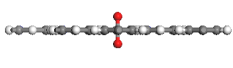
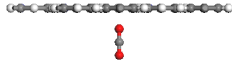
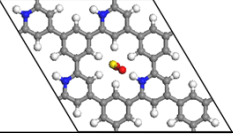
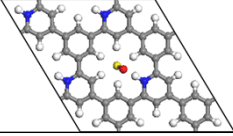
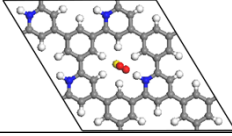
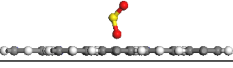
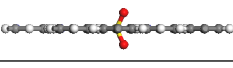
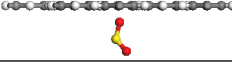
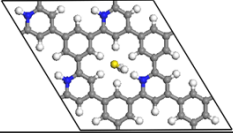
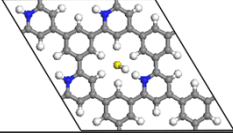
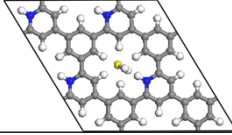
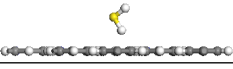
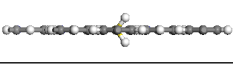
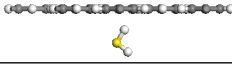
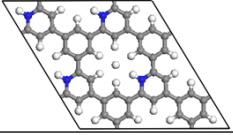
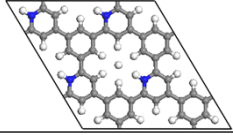
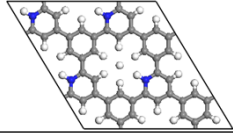
	Side view			
	Total energy	-2030.5086368	-2030.4376094	-2030.5086368
SO ₂	Top view			
	Side view			
	Total energy	-2390.4569014	-2390.3204854	-2390.4569013
H ₂ S	Top view			
	Side view			
	Total energy	-2241.2908148	-2241.1384297	-2241.2908148
HF	Top view			
	Side view			
	Total energy	-1942.4293529	-1942.3949017	-1942.4200398

Table S2 The initial, transition-state, and final configurations for the studied gases passing through 1N-PG, and their total energies are in Hartree. (C, gray; H, white; N, blue; O, red; Cl, light green; S, blue; F, light blue.)

Gas	Property	Initial State	Transition State	Final State
O ₂	Top view			
	Side view			
	Total energy	-2058.7470126	-2058.7451974	-2058.7470126
CO	Top view			
	Side view			
	Total energy	-2021.7456204	-2021.6634156	-2021.7411595

Cl ₂	Top view			
	Side view			
	Total energy	-2828.5679354	-2828.5037631	-2828.5679354
HCN	Top view			
	Side view			
	Total energy	-2001.8623352	-2001.7779916	-2001.8489644
NO	Top view			
	Side view			
	Total energy	-2038.3257654	-2038.2818481	-2038.3160590
CO ₂	Top view			
	Side view			
	Total energy	-2096.9893172	-2096.9106533	-2096.9893172
SO ₂	Top view			
	Side view			
	Total energy	-2456.9492844	-2456.8270763	-2456.9492846
H ₂ S	Top view			
	Side view			
	Total energy	-2307.7687776	-2307.6170446	-2307.7687774
HF	Top view			

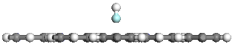
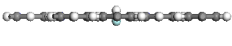

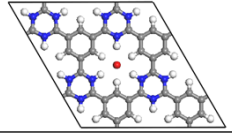
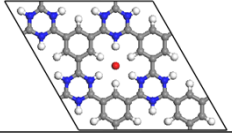
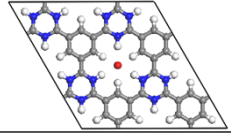
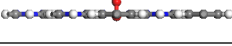
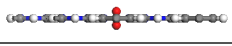
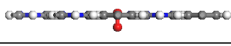
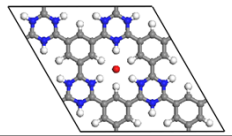
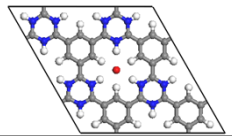
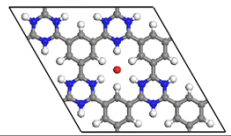
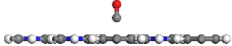
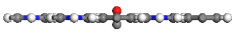
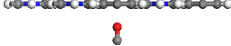
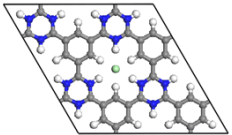
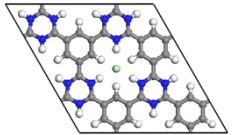
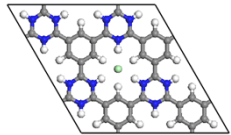

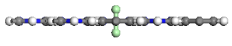

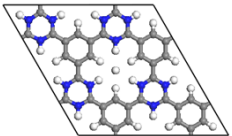
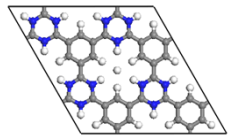
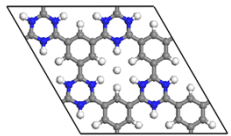


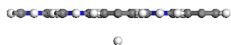
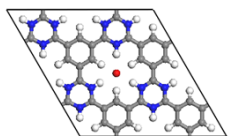
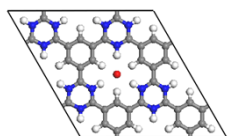
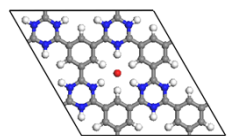

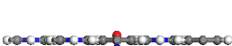
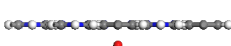
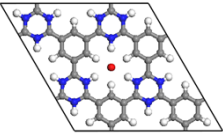
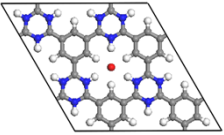
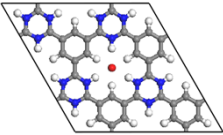
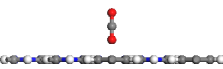
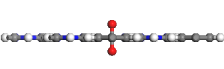
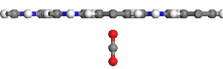
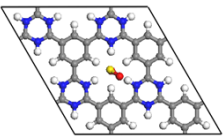
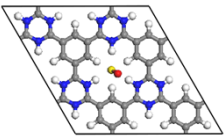
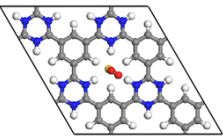

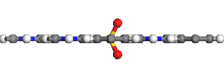
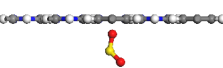
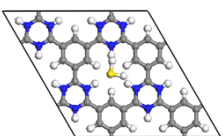
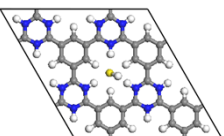
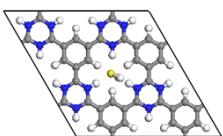
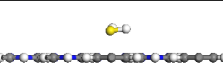
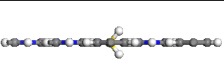
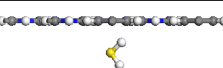
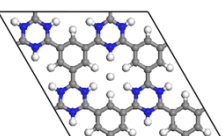
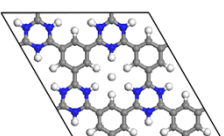
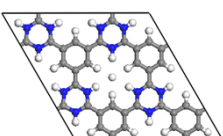
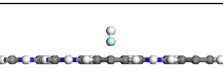
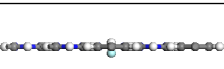
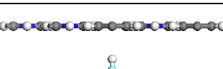
	Side view			
	Total energy	-2008.9103454	-2008.8738443	-2008.9000594

Table S3 The initial, transition-state, and final configurations for the studied gases passing through 3N-PG, and their total energies are in Hartree. (C, gray; H, white; N, blue; O, red; Cl, light green; S, blue; F, light blue.)

Gas	Property	Initial State	Transition State	Final State
O ₂	Top view			
	Side view			
	Total energy	-2191.7290054	-2191.7285522	-2191.7290054
CO	Top view			
	Side view			
	Total energy	-2154.7108589	-2154.6391155	-2154.7027929
Cl ₂	Top view			
	Side view			
	Total energy	-2961.5284954	-2961.4748779	-2961.5284954
HCN	Top view			
	Side view			
	Total energy	-2134.8266934	-2134.7557546	-2134.8092792
NO	Top view			
	Side view			
	Total energy	-2171.2963066	-2171.2649015	-2171.2808359

CO ₂	Top view			
	Side view			
	Total energy	-2229.9517056	-2229.8666913	-2229.9517056
SO ₂	Top view			
	Side view			
	Total energy	-2589.9118531	-2589.8002750	-2589.9118641
H ₂ S	Top view			
	Side view			
	Total energy	-2440.7401399	-2440.6040695	-2440.7279691
HF	Top view			
	Side view			
	Total energy	-2141.8733519	-2141.8372663	-2141.8601663