A promising monolayer membrane for oxygen separation

from harmful gases: Nitrogen-substituted polyphenylene

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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.)

Gas	Property	Initial State	Transition State	Final State
O ₂	Top view			
	Side view	\$ 09-0-009-0-009-0-009-0-000	6 0-C-830-C-830<mark>-</mark>8430-C-830-0 -0C	00-0-660-0-660-0-660-0-600
	Total energy	-1992.2389698	-1992.1978962	- 1992.2389698
СО	Top view			
	Side view	8 60-0-600-0-600-0-600-0-600-0-00	69-0-609-0-609 <mark>-</mark> 603-0-609-9-0	60-6-660-6-660-660-6-660-66 8
	Total energy	-1955.2642203	-1955.1787357	-1955.2608557
Cla	Top view			
	Side view	0 69-0-669-0-663-0-663-0-663-0-6	00-0-800-0-8000-800-0-800-0-800-0-800-	00
	Total energy	-2762.0788987	-2761.9895108	-2762.0788987
HCN	Top view			
	Side view	0 60-0-660-0-660-0-660-0-660-0-66	0 0-0-609-0-609<mark>-</mark>-609-0-60 0	69-0-669-0-669-0-669-0-669-0-66 0 0
	Total energy	-1935.3811051	-1935.2938272	-1935.3690994
NO	Top view			
	Side view	1 0 0-043-043-043-04 3	60-0-60 0-0-600-<mark>9-</mark>660-0-600 -0-00	69-6-819-6-819-0-863-6-819-0-86 \$
	Total energy	-1971.8339982	-1971.7650242	-1971.8309752
CO ₂	Top view			

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, bule; F, light blue.)

	Side view	60-0-680-0-630-0-630-0-60	0 0-0-660-0-660-0-660-0-6 0	00-0-660-0-660-0-660-0-660-0-60 8
	Total energy	-2030.5086368	-2030.4376094	-2030.5086368
SO_2	Top view			
	Side view	\$ \$\$\$\$-\$\$\$\$-\$\$\$\$-\$\$\$	00-040-040-040-040-040-060	60-0-660-0-660-0-660-0-660-0-60 }
	Total energy	-2390.4569014	-2390.3204854	-2390.4569013
H_2S	Top view			
	Side view	\$ (0-0-60-0-60-60-60-60-60-60-60-60-60-60-6		6 010120-1 60120-10-
	Total energy	-2241.2908148	-2241.1384297	-2241.2908148
HF	Top view			
	Side view	6 (10-C-818-C-818-0-812-C-818-0-8C	00-0-889-0-838- <u>8</u> -863-0-860-000	0 0-0-600-0-600-0-600-0-600 -0- 6 00-0-600-0600-00-
	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, bule; F, light blue.)

Gas	Property	Initial State	Transition State	Final State
O ₂	Top view			
	Side view	60-0-808-0-803-0-803-0-90	6 60-660-660<mark>-</mark>660-660-6 0	60-0409-0409-0409-0409-0-00
	Total energy	-2058.7470126	-2058.7451974	-2058.7470126
СО	Top view			
	Side view	8 (0-0-6630-0-6630-0-6630-0-6630-0-66	690-6000-600\$600-600	00-0-660-0-660-0-660-0-600 8
	Total energy	-2021.7456204	-2021.6634156	-2021.7411595

Cl ₂	Top view			
	Side view	00-0- 610-0-610-0-610-0-6 00		00-0-850-0-80-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-850-0-800-0-800-0-800-0-800-0-800-0-800-0-850-0-80
	Total energy	-2828.5679354	-2828.5037631	-2828.5679354
HCN	Top view			
	Side view	60-0-468-0-468-0-468-0-468-0-00	60-0-669-0-662 <mark>9</mark> -662-0-669-0-60	00-0-888-0-888-0-888-0-888-0-868 0 0 0
	Total energy	-2001.8623352	-2001.7779916	-2001.8489644
NO	Top view			
	Side view	6 0-0- 669-0-669-0-669-0-669-0-6 00	99-0- 639-0-639<mark>8</mark>463-0-639-0- 00	60-0-460-0-460-0-460-0-00
	Total energy	-2038.3257654	-2038.2818481	-2038.3160590
CO	Top view			
	Side view	60-0-880-0-880-0-880-0-880-0-00	60-0-650-0-6530-0-6530-0-60	90-0-860-0-860-0-860-0-860-0-00 0
	Total energy	-2096.9893172	-2096.9106533	-2096.9893172
SO ₂	Top view			
	Side view	60-0-600-0-600-0-600-0-600	00-000-000-000-000	00-0400-400-400-400-400-400
	Total energy	-2456.9492844	-2456.8270763	-2456.9492846
H ₂ S	Top view			
	Side view	60-0-660-0-660-0-660-0-60		60-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880-0-880
	Total energy	-2307.7687776	-2307.6170446	-2307.7687774
HF	Top view			

Side view	8 60-0-460-0-460-0-460-0-460-0-00	00-0400-000-040-040-040-040-040-040-040	60-0-669-0-669-0-669-0-669-0-60 8
 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, bule; F, light blue.)

0 0		,		
Gas	Property	Initial State	Transition State	Final State
O ₂	Top view			
	Side view	6 0-C-EED-C-EED-<mark>0</mark>-BE3-C-EED-0-0 -C	(00-200-20<mark>8</mark>53-20 0-00)	(0)(-E(0)(-E[0]0<mark>0</mark>0(0)(-E[0-0 -0))
	Total energy	-2191.7290054	-2191.7285522	-2191.7290054
0	Top view			
	Side view	8 6 0-0-880-0-880-0-880-0-8 00-0-00	6 0-0-€60-0-€20∯-8€3-0-8 €0	00-0-408-0-408-0-408-0-408-0-40 8
	Total energy	-2154.7108589	-2154.6391155	-2154.7027929
Cla	Top view			
	Side view	0 60-0-610-0-610-0-60	(9)(- 6(9)(-6(3)(-6(3)-6-9 ()	69-0-659-0-659-0-659-0-650 0
	Total energy	-2961.5284954	-2961.4748779	-2961.5284954
HCN	Top view			
	Side view	0 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	(0-C-E(0-C-E)) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	60-0-660-0-660-0-660-0-00 0 0 0
	Total energy	-2134.8266934	-2134.7557546	-2134.8092792
NO	Top view			
	Side view	\$ (0-0-610-0-610-0-610-0-00	0 0-0-669-0-613-<mark>0</mark>-663-0-0 0	00-0-860-0-860-0-860-0-860-0-860 8
	Total energy	-2171.2963066	-2171.2649015	-2171.2808359

CO ₂	Top view			
	Side view	69-6-469-6-463-6-463-6-66	69 	69-0-829-0-829-0-829-0-829-0-80 0
	Total energy	-2229.9517056	-2229.8666913	-2229.9517056
SO ₂	Top view			
	Side view	00EDEDEDEDEDED	6 86-689-6-619-682-6-619-0-8 0	000-ED-0-ED-0-ED-0-ED-0-ED-0-ED-0-ED-0-
	Total energy	-2589.9118531	-2589.8002750	-2589.9118641
H ₂ S	Top view			
	Side view	€-0 0 00-459-0-639-0-663-0-0 0	000-2000-200	600-E00-ED-0ED-0-ED-0-C 6
	Total energy	-2440.7401399	-2440.6040695	-2440.7279691
HF	Top view			
	Side view	69-0-469-0-463-0-463-0-60	690-8890-813- <u>8</u> 829-0-813-0-80	60-0-880-0-880-0-880-0-880-0-80 8
	Total energy	-2141.8733519	-2141.8372663	-2141.8601663