

Supporting Information

Functionalized GO membranes for efficient separation of acid gases from natural gas: a computational mechanistic understanding

Quan Liu¹, Zhonglian Yang^{1,*}, Gongping Liu², Longlong Sun¹, Rong Xu^{3,*}, and Jing Zhong³

¹ Analytical and Testing Center, School of Chemical Engineering, Anhui University of Science and Technology, Huainan 232001, China

² State Key Laboratory of Materials-Oriented Chemical Engineering, College of Chemical Engineering, Nanjing Tech University, 30 Puzhu Road (S), Nanjing 211816, China

³ Key Laboratory of Advanced Catalytic Materials and Technology, School of Petrochemical Engineering, Changzhou University, Gehu Road, 213164 Changzhou, China

* Correspondence: zhlyang@aust.edu.cn (Z.Y.); gpliu@njtech.edu.cn (G.L.); xurong@cczu.edu.cn (R.X.)

1. Fitting parameters of unary isotherms with variable adsorption models

Table S1 Fitting parameters of α , γ , β , n and correlation coefficient (R^2) for adsorption isotherms of different gases.

Gases	β	γ	n	R^2
GO without PDASA				
N ₂	0.001282391	0.000223	1	0.999
CH ₄	0.002666389	0.000329		0.999
CO ₂	3.390677	1.56608	0.90293	0.994
H ₂ S	3.859465	1.49488	0.91607	0.995
GO-1.5wt% PDASA				
N ₂	0.003777	0.00138	1	0.999
CH ₄	0.011565	0.00379		0.999
CO ₂	4.295758	1.56059	0.90492	0.997
H ₂ S	4.731904	1.16065	0.96424	0.992
GO-3.0wt% PDASA				
N ₂	0.003449	0.00126	1	0.999
CH ₄	0.010963	0.00343		0.999
CO ₂	4.518861	2.49722	0.82063	0.992
H ₂ S	5.258144	1.72125	0.89405	0.994
GO-4.5wt% PDASA				
N ₂	0.003589	0.00131	1	0.999
CH ₄	0.012041	0.00394		0.999
CO ₂	3.694794	2.27132	0.83429	0.989
H ₂ S	4.789341	1.53676	0.91312	0.996
GO-6.0wt% PDASA				
N ₂	0.003887	0.00159	1	0.999
CH ₄	0.013281	0.00473		0.999
CO ₂	3.811163	2.12759	0.85396	0.994
H ₂ S	4.2226	1.29829	0.94332	0.998
GO-7.5wt% PDASA				
N ₂	0.003946	0.0016	1	0.999
CH ₄	0.013637	0.00492		0.999
CO ₂	3.187251	1.37293	0.88646	0.993
H ₂ S	3.697801	1.07954	0.94362	0.995

2. Logarithmic form of MSD-t curves

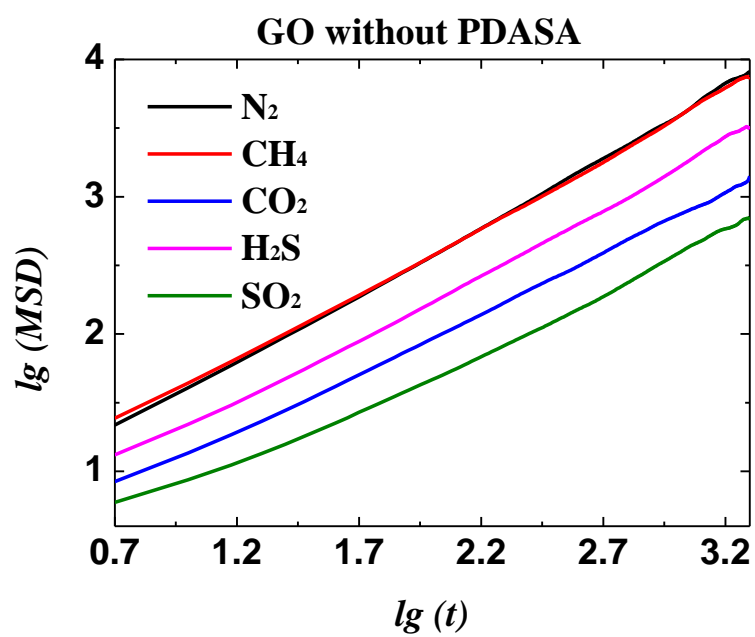


Figure S1. The $\lg(MSD)$ - $\lg(t)$ curve for the transport of variable gases through pure GO and GO-7.5wt%PDASA membranes.

3. Separation performance of different gas through GO membranes

Table S2 The solubility coefficient, diffusion coefficient and permeability with the typically reported unit.

Gases	S ($\text{cm}^3(\text{STP})\cdot\text{cm}^{-3}\cdot\text{mmHg}$)	D ($10^{-7} \text{ cm}^2\cdot\text{s}^{-1}$)	P (Barrer)
GO without PDASA			
N ₂	0.099598	699.9205	69.710
CH ₄	0.299538	662.4247	198.42
CO ₂	91.00181	150.2325	13671.42
H ₂ S	103.5835	210.2658	21780.07
GO-1.5wt% PDASA			
N ₂	0.102874	553.2705	56.92
CH ₄	0.315006	547.9411	172.60
CO ₂	117.0023	141.2156	16522.55
H ₂ S	128.8815	198.2641	25552.57
GO-3.0wt% PDASA			
N ₂	0.092981	458.2813	42.61
CH ₄	0.300666	443.8846	133.46
CO ₂	124.8961	93.3594	11660.22
H ₂ S	145.329	146.3784	21273.03
GO-4.5wt% PDASA			
N ₂	0.10064	280.9014	28.27
CH ₄	0.337283	253.8995	85.64
CO ₂	103.5978	70.132	7265.52
H ₂ S	134.2876	128.0338	17193.36
GO-6.0wt% PDASA			
N ₂	0.110555	288.3706	31.88
CH ₄	0.37771	252.1763	95.25
CO ₂	108.3851	37.7374	4090.17
H ₂ S	120.0859	78.1211	9381.25
GO-7.5wt% PDASA			
N ₂	0.113789	230.3564	26.21
CH ₄	0.393263	219.3084	86.25
CO ₂	91.91672	20.6643	1899.40
H ₂ S	106.6404	16.8647	1798.46

4. Performance comparison

Table S3 Performance comparison for separations of CO₂/CH₄ and (CO₂+H₂S)/CH₄.

P _{CO2} (Barrer)	$\alpha_{\text{CO}_2/\text{CH}_4}$	P _(CO2+H2S) (Barrer)	$\alpha_{(\text{CO}_2+\text{H}_2\text{S})/\text{CH}_4}$	Reference
864	30.7	1180	42	[1]
547	28.2	948	48.9	[2]
599	23.8	1047	42.4	
385	15.2	737	29	[3]
193	18.2	365	34.4	
84.3	24.4	152.3	44	[4]
92	14.9	228	40.9	[5]
76.1	14.2	188.1	35.2	[6]
26	22.3	52.5	45	[7]
142.2	10.35	418	30.43	[8]
100.2	15.24	262.7	39.96	
332	25.7	914.9	40.5	[9]
246.5	26.5	682.4	41.4	
206.9	30	582.2	46.6	
495.1	19	796.1	50.2	
473.5	24.4	671.8	39.7	[10]
496.3	25	823.2	41.5	
543.2	27.1	936.2	46.7	
587.9	29.3	1057.7	52.8	
432.8	26.3	702.3	42.5	
460.4	30.3	747.8	49.2	
460.4	30.3	137.9	52.1	
95.6	36.1	196.1	56.2	
135	38.7	225.9	66.1	
11660.2	87.4	32933.3	246.8	GO-3.0wt% PDASA (This work)
7265.5	84.8	24458.9	285.7	GO-4.5wt% PDASA (This work)

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