SUPPLEMENTARY INFORMATION

"ZIF-95 as a Filler for Enhanced Gas Separation Performance of Polysulfone Membrane"

Sanaullah Shafiq ^a, Bassem A. Al-Maythalony ^{b, c}, Muhammad Usman ^d, Mohammad Saleh Ba-Shammakh ^a, Abdallah A. Al-Shammari ^{a,*}

^a Chemical Engineering Department, King Fahad University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia.

^b King Abdulaziz City for Science and Technology—Technology Innovation Centre on Carbon Capture and Sequestration (KACST-TIC on CCS) at King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia.

^c Material Discovery Unit-Research and Development, Royal Scientific Society (RSS), Amman 11941, Jordan.

^d Center of Research Excellence in Nanotechnology, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia.

*Correspondence should be addressed at: alshammari@kfupm.edu.sa

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S1. CO₂ Adsorption Isotherm of ZIF-95:



Fig. S1. Adsorption and desorption isotherms of CO₂ at 273 K (blue), 293 K (green), and 313 K (red) for synthesized ZIF-95.

Clausius-Clapeyron equation:

Where, Qst is the isosteric heat of adsorption in kJ/mol, R is the general gas constant (kJ/mol.K), p is the relative pressure, and T is the temperature (Kelvin).

S2. Activation Procedure:

Acetone was used to solvent exchange the DMF from ZIF-95 crystals. As-synthesized sample was immersed in acetone for 5 days during which acetone was refreshed 2 to 3 times in a day. Afterward, the crystals of ZIF-95 were partially dried overnight in the fume hood. The degassing of the partially dried sample was done using a vacuum degassing option on Autosorb iQ equipment. The sample was first heated to 50 °C for 10 hours and then to 110 °C for 12 hours under vacuum.

S3. Permeability calculations:

Where, Pi is the permeability of gas "*i*" in "Barrer", L is the thickness of membrane in "*cm*", Δp is the pressure difference across the membrane in "*cmHg*", and *Fi* is the flux of gas "*i*". The flux of gas "*i*" was calculated using the following equation:

$$F_i = 10^{10} \left(\frac{dp_d^{SS}}{dt} - \frac{dp_d^{LR}}{dt} \right) \cdot V_d \cdot ART \dots \dots \dots \dots \dots \dots \dots (eq.S3)$$

where,

 $\begin{array}{l} A = Area \ of \ membrane \ (cm^2) \\ Vd = Volume \ of \ down \ stream \ (cm^3) \\ R = \ General \ gas \ constant \ [\ 0.278 \ cm3 \ cmHg/(cm3(STP)K \] \\ T = \ Temperature \ (Kelvin) \\ \\ \frac{dp_d^{SS}}{dt} = Pressure \ rise \ in \ down \ stream \ at \ steady \ state \ (cmHg/s) \\ \\ \frac{dp_d^{LR}}{dt} = Leak \ rate \ on \ the \ down \ stream \ (cmHg/s) \end{array}$



Fig. S2. The schematic diagram of permeation setup.

S4. EDS Mapping of Cross-Section:



Fig. S3. EDX mapping (Zinc) of PSF-ZIF-95-8% loaded membrane (yellow), PSF-ZIF-95-16% loaded membrane (purple), PSF-ZIF-95-24% loaded membrane (green), and PSF-ZIF-95-32% loaded membrane (red).

S5. DSC Data of Membranes:



Fig. S4. DSC thermograms of pure and loaded mixed matrix membranes

S6. Permeabilities & Selectivity:

Note: In all the tables, permeabilities and permeances are provided Barrer and GPU units, respectively.

 Table S1. Permeability of synthesized membranes.

MFMBRANF	Permeability (Barrer)											
MEMDRANE	Helium	Hydrogen	Oxygen	Carbon dioxide	Nitrogen	Methane						
Polysulfone Pure	9.34	9.60	0.91	4.88	0.160	0.160						
Polysufone-ZIF-95 (8%)	10.2	11.28	1.03	5.50	0.160	0.160						
Polysufone-ZIF-95 (16%)	12.04	13.14	1.23	6.47	0.195	0.186						
Polysufone-ZIF-95 (24%)	15.21	17.30	1.62	8.16	0.256	0.250						
Polysufone-ZIF-95 (32%)	17.68	21.14	2.19	11.11	0.399	0.390						

 Table S2. Selectivity of synthesized membranes.

MEMBRANE		Ideal Selectivity														
	He/H ₂	He/O ₂	He/CO ₂	He/N ₂	He/CH ₄	H ₂ /O ₂	H ₂ /CO ₂	H_2/N_2	H ₂ /CH ₄	CO ₂ /N ₂	CO ₂ /CH ₄	O ₂ /N ₂	N ₂ /CH ₄			
Polysulfone Pure (0 %)	0.972	10.263	1.913	58.375	58.375	10.549	1.967	60.000	60.000	30.500	30.500	5.687	1.000			
Polysufone-ZIF-95 (8%)	0.904	9.902	1.854	63.750	63.750	10.951	2.050	70.500	70.500	34.375	34.375	6.437	1.000			
Polysufone-ZIF-95 (16%)	0.916	9.788	1.860	61.743	64.731	10.682	2.030	67.384	70.645	33.179	34.784	6.307	1.048			
Polysufone-ZIF-95 (24%)	0.879	9.388	1.864	59.414	60.840	10.679	2.120	67.578	69.200	31.875	32.640	6.328	1.024			
Polysufone-ZIF-95 (32 %)	0.836	8.073	1.5632	44.310	45.333	9.652	1.902	52.982	54.205	27.844	28.487	5.488	1.023			

S7. Diffusivity and Solubility

Membrane	D_He	D_H ₂	D_O ₂	D_CO ₂	D_N ₂	D_CH4
Pure PSF	1.08×10 ⁻⁷	5.6×10 ⁻⁸	1.53×10 ⁻⁸	6.61×10-9	2.39×10 ⁻⁹	1.98×10 ⁻⁹
PSF-ZIF-95-8%	1.46×10 ⁻⁷	1.09×10 ⁻⁸	1.80×10 ⁻⁸	7.78×10-9	2.89×10-9	1.95×10-9
PSF-ZIF-95-16%	2.05×10 ⁻⁷	2.29×10 ⁻⁷	2.25×10 ⁻⁸	1.13×10 ⁻⁸	4.43×10 ⁻⁹	2.07×10 ⁻⁹
PSF-ZIF-95-24%	3.17×10 ⁻⁷	3.70×10 ⁻⁷	2.93×10 ⁻⁸	1.41×10 ⁻⁸	6.27×10 ⁻⁹	2.41×10-9
PSF-ZIF-95-32%	4.01×10 ⁻⁷	5.77×10 ⁻⁷	3.94×10 ⁻⁸	2.15×10 ⁻⁸	9.8×10-9	3.10×10 ⁻⁹

 Table S3. Diffusivity coefficients (cm²/s) of Pure and loaded mixed matrix membranes.

MEMBRANE						Diffu	isivity Sele	ctivity					
Table S3 (continued)	He/H ₂	He/O ₂	He/CO ₂	He/N ₂	He/CH ₄	H ₂ /O ₂	H_2/CO_2	H_2/N_2	H ₂ /CH ₄	CO ₂ /N ₂	CO ₂ /CH ₄	O_2/N_2	N ₂ /CH ₄
Polysulfone Pure (0 %)	1.926	7.051	16.320	45.038	54.486	3.660	8.472	23.378	28.283	2.760	3.339	6.387	1.210
Polysufone-ZIF-95 (8%)	1.338	8.114	18.763	50.614	74.900	6.063	14.021	37.821	55.968	2.698	3.992	6.238	1.480
Polysufone-ZIF-95 (16%)	0.892	9.107	18.202	46.244	98.934	10.204	20.395	51.815	110.853	2.541	5.435	5.078	2.139
Polysufone-ZIF-95 (24%)	0.857	10.823	22.427	50.615	131.748	12.622	26.155	59.027	153.646	2.257	5.874	4.676	2.603
Polysufone-ZIF-95 (32%)	0.695	10.163	18.673	40.839	129.311	14.620	26.862	58.750	186.022	2.187	6.925	4.018	3.166

Membrane	S_He	S_H ₂	S_O ₂	S_CO ₂	S_N ₂	S_CH ₄
Pure PSF	8.67×10 ⁺⁷	1.74 ×10 ⁺⁸	5.73×10 ⁺⁷	7.36×10 ⁺⁸	7.18×10 ⁺⁷	8.43×10 ⁺⁷
PSF-ZIF-95-8%	7.05×10 ⁺⁷	$1.03 \times 10^{+8}$	5.87×10 ⁺⁷	$7.10 \times 10^{+8}$	6.32 ×10 ⁺⁷	8.67 ×10 ⁺⁷
PSF-ZIF-95-16%	5.85×10 ⁺⁷	5.63×10 ⁺⁷	5.32×10 ⁺⁷	5.59×10 ⁺⁸	5.56×10 ⁺⁷	9.38×10 ⁺⁷
PSF-ZIF-95-24%	4.79×10 ⁺⁷	4.67×10 ⁺⁷	5.60×10 ⁺⁷	5.75×10 ⁺⁸	4.46×10 ⁺⁷	1.08×10 ⁺⁸
PSF-ZIF-95-32%	4.44×10 ⁺⁷	3.64×10 ⁺⁷	5.36×10 ⁺⁷	5.14×10 ⁺⁸	4.04×10 ⁺⁷	1.10×10 ⁺⁸

Table S4. Solubility coefficients [Unit = cm^3 (gas) cm^{-3} (ZIF) cmHg] of bare and loaded mixed matrix membrane.

MEMBRANE		Solubility Selectivity											
Table S4(Continued)	He/H ₂	He/O ₂	He/CO ₂	He/N ₂	He/CH4	H ₂ /O ₂	H ₂ /CO ₂	H_2/N_2	H ₂ /CH ₄	CO ₂ /N ₂	CO ₂ /CH ₄	O ₂ /N ₂	N ₂ /CH ₄
Polysulfone Pure (0 %)	0.498	1.513	0.117	1.207	1.028	3.036	0.236	2.422	2.064	10.249	8.732	0.797	0.852
Polysufone-ZIF-95 (8%)	0.681	1.201	0.099	1.115	0.813	1.762	0.145	1.635	1.193	11.222	8.184	0.928	0.729
Polysufone-ZIF-95 (16%)	1.038	1.098	0.104	1.052	0.623	1.057	0.100	1.013	0.600	10.061	5.959	0.957	0.592
Polysufone-ZIF-95 (24%)	1.025	0.856	0.083	1.074	0.443	0.834	0.081	1.047	0.432	12.907	5.322	1.255	0.412
Polysufone-ZIF-95 (32 %)	1.220	0.829	0.086	1.099	0.400	0.679	0.070	0.901	0.327	12.727	4.631	1.325	0.363

S8. Literature of Mixed Matrix Membranes (Reporting permeabilities except where permanence is mentioned)

Table S5. Literature review of MMMs reported for He, H₂, O₂, CO₂, N₂, and CH₄ gases separation.

MEMBRANE	YEAR	Temperature	Helium	Hydrogen	Oxygen	Carbon dioxide	Nitrogen	Methane	Ref
PSF	2006	35 C (4 Bar)	8.02		0.89	4.46	0.18	0.17	1
PSF/MCM-48 (20%)			32.1		4.14	18.21	0.77	0.77	
Matrimid 5218	2011	35 C (3 Bar)	8.75		1.29	4.3	0.22	0.21	2
Matrimid/TiO ₂ (20 %)			19		2.45	10.54	0.92	0.77	
Matrimid 5218	2012	22 C (4 Bar)		32.68	2.62	8.07	0.36	0.23	3
Matrimid/ZIF-8 (20%)				63.53	5.63	16.63	0.88	0.46	
PEI	2014	25 C (6 Bar)		10.07		1.68	0.1	0.09	4
PEI/MOF-5 (25%)				28.32		5.39	0.19	0.23	
PIM-1	2016	25 C (5 Bar)	1170	2710	875	4770	219	286	5
PIM-1/UiO-66-NH2 (16.6 %)			1340	3130	1090	6340	303	425	
PIM-1	2016	25 C (2 Bar)		32.68	2.62	8.07	0.36	0.23	6
PIM/Mg-MOF-74 (20 %)				63.53	5.63	16.63	0.88	0.46	
PEI	2017	35 C (2 Bar)		856	119.9	82.5	21.8	18.9	7
PEI/nZIF-7-PSM (5%)				2020	272.9	245.9	182.6	107.9	
Akram PI spongy	2019	35 C (2 Bar)		128.7 (Permeance)	16.8 (Permeance)	69.1 (Permeance)	4.3 (Permeance)	4.1 (Permeance)	8
Akram PI/ZIF-302 (5%)				156.4 (Permeance)	14.1 (Permeance)	62 (Permeance)	2.5 (Permeance)	3.7 (Permeance)	

Table S5 Continued]	deal Selectivi	ity					
Membrane	He/H ₂	He/O ₂	He/CO ₂	He/N ₂	He/CH4	H ₂ /O ₂	H ₂ /CO ₂	H ₂ /N ₂	H ₂ /CH ₄	CO ₂ /N ₂	CO ₂ /CH ₄	O ₂ /N ₂	N ₂ /CH ₄
PSF		8.183	1.798	44.555	47.176					24.777	26.235	5.444	1.058
PSF/MCM-48 (20%)		7.753	1.762	41.688	41.688					23.649	23.649	5.376	1.000
Matrimid 5218		6.782	2.034	39.772	41.666					19.545	20.476	5.863	1.047
Matrimid/TiO ₂ (20 %)		7.755	1.802	20.652	24.675					11.456	13.688	2.663	1.194
Matrimid 5218						12.473	4.049	90.777	142.087	22.416	35.087	7.277	1.565
Matrimid/ZIF-8 (20%)						11.284	3.820	72.193	138.108	18.897	36.152	6.397	1.913
PEI							5.994	100.700	111.888	16.800	18.666		1.111
PEI/MOF-5 (25%)							5.254	149.052	123.130	28.368	23.434		0.826
PIM-1	0.431	1.337	0.245	5.342	4.090	3.097	0.568	12.374	9.475	21.780	16.678	3.995	0.765
PIM-1/UiO-66-NH2 (16.6 %)	0.428	1.229	0.211	4.422	3.152	2.871	0.493	10.330	7.364	20.924	14.917	3.597	0.712
PIM-1						3.299	0.537	10.076	6.598	18.73	12.268	3.054	0.654
PIM/Mg-MOF-74 (20 %)						5.095	0.539	15.456	10.295	28.664	19.092	3.033	0.666
PEI						7.139	10.375	39.266	45.291	3.784	4.365	5.500	1.153
PEI/nZIF-7-PSM (5%)						7.405	8.218	11.067	18.729	1.346	2.279	1.494	1.692
PI						7.660	1.862	29.930	31.390	16.069	16.853	3.907	1.048
PI/ZIF-302 (5%)						11.092	2.522	62.560	42.270	24.800	16.756	5.640	0.675

MEMBRANE	YEAR	Temperature	Oxygen	Carbon dioxide	Nitrogen	Methane	CO ₂ /N ₂	CO ₂ /CH ₄	O_2/N_2	N ₂ /CH ₄	Ref.
PSF	1996	35 C (10 Bar)	1.29	5.5	0.22	0.24	25.000	22.916	5.863	0.916	9
PSF-HN2-16%			0.69	2.7	0.11	0.11	24.545	24.545	6.272	1.000	
PSF	2001	35 C (3 Bar)	1.5	7.53	0.257	0.389	29.299	19.357	5.836	0.660	10
PSF/MCM-41 (30%)			3.83	20.5	0.753	1.05	27.224	19.523	5.086	0.717	
PSF	2011	25 C (4 Bar)	2.75	16	0.47	0.45	34.042	35.555	5.851	1.044	11
PSF/MCM41-APTMS- Modified (20 %)			4.04	23	0.52	0.52	44.230	44.230	7.769	1.000	
PSF	2011	35 C (3.5Bar)	1.107	2	0.402	0.484	4.975	4.125	2.753	0.829	12
PI			0.727	1.595	0.2403	0.361	6.641	4.413	3.027	0.664	
PSF-PI/ZSM-5 (20%)			0.876	1.528	0.2943	0.349	5.194	4.379	2.978	0.843	
PSF	2012	30 C (3 Bar)	1.47		0.25				5.88		13
PSF/MIL-101(Cr) (8%)			2.53		0.47				5.383		
PSF/MIL-101(Fe) (8%)			2.03		0.35				5.80		
PSF	2016	35 C (3 Bar)		5.6	0.19	0.21					14
PSF/NH2-UiO-66 (50%)				43	1.65	1.8					
PSF	2017	35 C (3 Bar)		5.6 (Permeance)	0.91 (Permeance)	1.73 (Permeance)	6.153	3.237			15
PSF/SAPO-34-IL6 (5%)				7.24 (Permeance)	0.38 (Permeance)	0.36 (Permeance)	19.052	20.111			

Table S6. Literature review of MMMs reported for O₂, CO₂, N₂, and CH₄ gases separation.

Table S6 Continued	Year	Temperature	Oxygen	Carbon	Nitrogen	Methane	CO ₂ /N ₂	CO ₂ /CH ₄	O ₂ /N ₂	N ₂ /CH ₄	Ref.
											<u> </u>
PSF	2011	35 C (2.75 Bar)	1.6		0.28				5.7143		16
PSF/ZIF-8 (16%)			2.6		0.31				8.3871		1
PES/MWCNT(Purified) (1%)	2011	27 C (3 Bar)	2.319	7.742	0.91	0.396	8.507	19.550	2.5484	2.2980	17
PES/MWCNT (Aptes Modified 1%)			3.178	2.794	0.511	0.09	5.467	31.044	6.2192	5.6778	1
PSF	2019	25 C (10 Bar)		6.18	0.21	0.22	29.428	28.090		0.9545	18
PSF/Bio-MOF-1 (30%)				16.57	0.36	0.39	46.027	42.487		0.9231	1
РІ	2018	25 C (1 Bar)	27.8	125.4	5.49	3.12	22.841	40.192	5.0638	1.7596	19
PI/ZIF-L (20%)			30.9	19.4	6.29	4.23	3.084	4.586	4.9126	1.4870	+
Matrimid 5218	2015	35 C (10 Bar)		4.44	0.131	0.126	33.893	35.238		1.0397	20
Matrimid /MIL-101(Cr) (10 %)				6.95	0.12	0.12	57.916	57.916		1.0000	1
6FDA-DAM	2018	24 C (4 Bar)		770	32.08		24.00				21
6FDA-DAM/ ZIF-94 (40%)				2310	105		22.00				1
PEBAX	2017	0 C (1 Bar)		53.7	1.79	3.00	30.00	17.900		0.5967	22
PEBAX/ ZIF-8 (15%) IL-(80%)				231.4	8.57	19.6	27.001	11.806		0.4372	1
Matrimid-PBI (3:1)	2021	22 C (10 Bar)	1.6	8.0	0.24		33.00				23
Matrimid-PBI (3:1)/ZIF-95X (20%)			0.78	3.1	0.16		19.38				1

MEMBRANE	YEAR	Temperature	Carbon dioxide	Nitrogen	Methane	CO ₂ /N ₂	CO ₂ /CH ₄	N ₂ /CH ₄	Ref.
PSF	2011	35 C (2.75 Bar)	5.95	0.24		24.791			16
PSF/Silicate-1-HKUST-(16%)			8.9	0.22		40.454			
PSF	2011	35 C (2.75 Bar)	4.6		0.19		24.210		16
PSF/Silicate-1-HKUST-(16%)			8.9		0.39		22.820		
PSF	2016	35 C (2 Bar)	4.7		0.21		22.38		24
PSF/ MIL-101(Cr)-ZIF-8 (16%)			14.2		0.35		40.57		
PSF	2016	25 C (2 Bar)	6.32	0.24		26.333			25
PSF/ZIF-301 (30%)			17.12	0.62		27.612			
PSF	2016	25 C (2 Bar)	6.32	0.24		26.333			26
PSF/GO-ZIF-301 (1%) (30%)			25	0.4		62.500			
PSF	2016	25 C (2 Bar)	6.32	0.24		26.333			27
PSFZIF-302-CNT-(12%) (8%)			18	0.514		35.019			
PSF	2016	25 C (2 Bar)	6.32	0.24		26.333			28
PSF/ZIF-302-GO (30%) (1%)			13.21	0.26		50.807			
PSF	2020	25 C (3 Bar)	10.75		0.354		30.367		29
PSF/ ZIF-11 (24%)			22.14		0.519		42.659		

Table S7. Literature review	of MMMs reported for	CO ₂ , N ₂ , and CH	I ₄ gases separation.
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Table S8. Literature review of MMMs reported for H_2 , CO_2 , N_2 , and CH_4 gases separation.

MEMBRANE	YEA R	Temperature	Hydrogen	Carbon dioxide	Methane	H ₂ /CO ₂	H ₂ /CH ₄	Ref.
PSF-acrylate	2010	25 C (12 Bar)	12.7 (Permeance)	8.19 (Permeance)		1.550		30
PSF/ APTMS- Zeolite-3A (30%)			14.78 (Permeance)	5.53 (Permeance)		2.672		
PSF	2011	35C (2.75 Bar)	11		0.19		57.89	16
PSF/ ZIF-8-(16%)			39.8		0.34		117.05	
PSF	2013	35 C (3 Bar)	8.2	3	0.27	2.733	30.37	31
PSF/SIO2-silanol modified (25%)			25	10.2	1.126	2.451	22.05	
РМР	2014	30 C (2 Bar)	11.14	98.74		0.112		32
PMP/ MIL-53(Al) (30%)			13.11	217.65		0.060		
PBI	2015	35 C (10 Bar)	3.62	0.4		9.05		33
PBI/[Cu2(ndc)2(d abco)]n (20%)			6.14	0.39		15.743		
PBI	2016	150 C (5 Bar)	30	7.89		3.802		34
PBI/ ZIF-8(10 %)			40	8.89		4.499		
Matrimid 5218	2018	35 C (7 Bar)		7.33	0.21		CO ₂ /CH ₄	35
							34.904	
PI-PVDF/ MIL- 101 (Cr) (10%)				14.87	0.24		CO ₂ /CH ₄ 61.958	
Matrimid	2021	35 C (7 Bar)	22.30	5.70	0.17		131.18	36
Matrimid/ZIF-95 (30%)			76.60	23.20	0.40		191.50	

S9. Upper Bounds:



Fig. S5. He/H₂ selectivity vs He permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S6. He/O₂ selectivity vs He permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S7. He/CO₂ selectivity vs He permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S8. He/N₂ selectivity vs He permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S9. He/CH₄ selectivity vs He permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S10. H_2/O_2 selectivity vs H_2 permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S11. H_2/CO_2 selectivity vs H_2 permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S12. H_2/N_2 selectivity vs H_2 permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S13. H_2/CH_4 selectivity vs H_2 permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S14. CO_2/N_2 selectivity vs CO_2 permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S15. CO_2/CH_4 selectivity vs CO_2 permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S16. O₂/N₂ selectivity vs O₂ permeability of Pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).



Fig. S17. N_2 /CH₄ selectivity vs N_2 permeability of pure membrane (blue), 8% loaded membrane (green), 16% loaded membrane (red), 24% loaded membrane (yellow), and 32% loaded membrane (purple).

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