Supporting Information: On the Importance of Non-Covalent Interactions for Porous Membranes: Unraveling the Role of Pore Size

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Table S1: Cartesian Coordinates (in Å) for C_2-square pore structure.

ATOM	X	Y	Z
C	0.865255478006	4.036263104154	0.000000000000
C	0.334137969934	2.703089490231	0.000000000000
C	0.058244520528	5.153927411934	0.000000000000
C	-1.363037718272	4.970764691184	0.000000000000
C	-1.860315949921	3.685013410455	0.000000000000
C	-1.008544675468	2.530059676958	0.000000000000
C	2.261158821749	3.453584970347	0.000000000000
C	1.686821457140	2.138455233993	0.000000000000
H	0.463462282670	6.159357766824	0.000000000000
H	-2.009925665278	5.840607877416	0.000000000000
C	3.623292213954	3.665804117747	0.000000000000
C	2.508012074287	1.062172137866	0.000000000000
C	4.492554503758	2.526519483510	0.000000000000
H	4.053152010145	4.660948204470	0.000000000000
C	3.928129870124	1.268796117040	0.000000000000
H	5.565892143195	2.678299563403	0.000000000000
C	4.121473652362	-0.231425667126	0.000000000000
C	2.695362023080	-0.391604054988	0.000000000000
C	2.173870079115	-1.640914146221	0.000000000000
C	4.986323831663	-1.304954389200	0.000000000000
C	3.062877663603	-2.767465949374	0.000000000000
C	4.434304849858	-2.627406146247	0.000000000000
H	6.063075327094	-1.179663576069	0.000000000000
H	5.102429793209	-3.481045896246	0.000000000000
C	1.008544675468	-2.530059676958	0.000000000000
C	1.860315949921	-3.685013410455	0.000000000000
C	-0.334137969934	-2.703089490231	0.000000000000
C	1.363037718272	-4.970764691184	0.000000000000
C	-0.865255478006	-4.036263104154	0.000000000000
C	-0.058244520528	-5.153927411934	0.000000000000
H	-0.463462282670	-6.159357766824	0.000000000000
H	2.009925665278	-5.840607877416	0.000000000000
C	-1.686821457140	-2.138455233993	0.000000000000
C	-2.261158821749	-3.453584970347	0.000000000000
C	-2.508012074287	-1.062172137866	0.000000000000
C	-3.623292213954	-3.665804117747	0.000000000000
C	-3.928129870124	-1.268796117040	0.000000000000
C	-4.492554503758	-2.526519483510	0.000000000000
H	-5.565892143195	-2.678299563403	0.000000000000
H	-4.053152010145	-4.660948204470	0.000000000000
C	-4.121473652362	0.231425667126	0.000000000000
C	-4.986323831663	1.304954389200	0.000000000000
C	-4.434304849858	2.627406146247	0.000000000000
C	-3.062877663603	2.767465949374	0.000000000000
H	-5.102429793209	3.481045896246	0.000000000000
H	-6.063075327094	1.179663576069	0.000000000000
C	-2.173870079115	1.640914146221	0.000000000000
C	-2.695362023080	0.391604054988	0.000000000000

Table S2: SAPT0/jun-cc-pVDZ energy components (kcal mol^{-1}) for the interaction between H_2 and the C_2-square pore structure.

Dist. (Å)	Elst.	Exch.	Ind.	Disp.	SAPT0
0.00	-6.44	16.54	-0.96	-6.94	2.21
0.20	-6.26	16.21	-0.95	-6.85	2.15
0.40	-5.74	15.26	-0.92	-6.59	2.00
0.60	-4.98	13.80	-0.88	-6.19	1.75
0.80	-4.10	11.99	-0.81	-5.69	1.39
1.00	-3.19	10.03	-0.73	-5.13	0.97
1.20	-2.36	8.07	-0.63	-4.56	0.53
1.40	-1.64	6.26	-0.52	-3.99	0.10
1.60	-1.08	4.69	-0.42	-3.46	-0.27
1.80	-0.65	3.39	-0.32	-2.97	-0.55
2.00	-0.35	2.38	-0.24	-2.53	-0.74
2.20	-0.15	1.62	-0.17	-2.14	-0.84
2.40	-0.03	1.07	-0.12	-1.80	-0.87
2.60	0.04	0.69	-0.08	-1.50	-0.85
2.80	0.07	0.44	-0.05	-1.25	-0.79
3.00	0.08	0.27	-0.03	-1.03	-0.71
3.20	0.07	0.16	-0.01	-0.85	-0.63
3.40	0.06	0.10	0.00	-0.70	-0.54
3.60	0.05	0.06	0.01	-0.58	-0.46
3.80	0.03	0.03	0.01	-0.47	-0.40
4.00	0.02	0.02	0.01	-0.39	-0.33
4.20	0.01	0.01	0.02	-0.32	-0.28
4.40	0.00	0.01	0.02	-0.26	-0.24
4.60	-0.01	0.00	0.02	-0.22	-0.20
4.80	-0.01	0.00	0.02	-0.18	-0.17
5.00	-0.01	0.00	0.02	-0.15	-0.15

Table S3: Cartesian Coordinates (in Å) for C_2-pent pore structure.

ATOM	X	Y	Z
C	-2.189244125710	3.734906942571	0.000000000000
C	-1.383160994944	2.359712861992	0.000000000000
C	-0.017497583141	2.659345365169	0.000000000000
C	-0.026721353701	4.061354736528	0.000000000000
C	1.163296536868	4.790596039857	0.000000000000
C	1.351985022618	2.377707274283	0.000000000000
C	2.139922464431	3.763433161606	0.000000000000
C	-0.741492141965	6.154093241051	0.000000000000
C	-1.226231179870	4.774858091878	0.000000000000
C	0.660442085893	6.163327556194	0.000000000000
C	2.294304962132	1.344829337093	0.000000000000
C	3.503866435444	2.053827788575	0.000000000000
C	4.730404160922	1.387857903224	0.000000000000
C	2.735149408625	0.017999915271	0.000000000000
C	4.329145910994	0.028490473586	0.000000000000
C	4.958855957593	3.719206653226	0.000000000000
C	3.522036065241	3.449393101854	0.000000000000
C	5.667804376787	2.509704269905	0.000000000000
C	1.383159556587	-2.359710516220	0.000000000000
C	2.189268549941	-3.734951511906	0.000000000000
C	3.567131194860	-3.402741952822	0.000000000000
C	3.530595617078	-2.007532918057	0.000000000000
C	4.748263012398	-1.325480265854	0.000000000000
C	5.007380494575	-3.653619240741	0.000000000000
C	5.700349361897	-2.434891045443	0.000000000000
C	2.311807263572	-1.314519208212	0.000000000000
C	-1.351986822841	-2.377718972817	0.000000000000
C	-2.139903902719	-3.763403233370	0.000000000000
C	-1.163285995281	-4.790585235901	0.000000000000
C	0.026732683015	-4.061360688619	0.000000000000
C	1.226245372683	-4.774878475096	0.000000000000
C	-0.660440434573	-6.163320875607	0.000000000000
C	0.741494637321	-6.154106709816	0.000000000000
C	0.017503245887	-2.659349868916	0.000000000000
C	-5.667819482811	-2.509699514402	0.000000000000
C	-4.958856084746	-3.719193146009	0.000000000000
C	-3.522034822580	-3.449371404358	0.000000000000
C	-3.503871828030	-2.053814590518	0.000000000000
C	-2.294305808124	-1.344825876307	0.000000000000
C	-4.329192347632	-0.028486255834	0.000000000000
C	-4.730424193123	-1.387851035647	0.000000000000
C	-2.735145836428	-0.017996501075	0.000000000000
C	-5.007370062157	3.653616265780	0.000000000000
C	-5.700353106034	2.434896199822	0.000000000000
C	-4.748277316237	1.325478754886	0.000000000000
C	-3.530597146140	2.007529958331	0.000000000000
C	-2.311808123865	1.314515580941	0.000000000000
C	-3.567122845395	3.402726676571	0.000000000000
H	6.748339645718	2.449777048381	0.000000000000
H	-1.252606976189	-7.069129090101	0.000000000000
H	-5.434475693311	-4.691271967224	0.000000000000
H	-5.495741357168	4.619350509908	0.000000000000
H	1.252599162309	7.069140512516	0.000000000000
H	-1.345527129564	7.052030100777	0.000000000000
H	-6.780006681911	2.360761011505	0.000000000000
H	-6.748356019223	-2.449779608688	0.000000000000
H	1.345521341848	-7.052048996082	0.000000000000
H	5.495759184502	-4.619350005409	0.000000000000
H	6.780003660725	-2.360748917094	0.000000000000
H	5.434480868661	4.691280038540	0.000000000000

Table S4: SAPT0/jun-cc-pVDZ energy components (kcal mol^{-1}) for the interaction between H_2 and the C_2-pent pore structure.

Dist. (Å)	Elst.	Exch.	Ind.	Disp.	SAPT0
0.00	-7.17	17.41	-1.20	-7.96	1.09
0.20	-6.95	17.10	-1.19	-7.85	1.11
0.40	-6.36	16.18	-1.15	-7.54	1.14
0.60	-5.48	14.76	-1.08	-7.07	1.13
0.80	-4.47	12.97	-0.98	-6.49	1.03
1.00	-3.45	10.98	-0.86	-5.86	0.81
1.20	-2.53	8.96	-0.73	-5.20	0.50
1.40	-1.76	7.05	-0.59	-4.56	0.13
1.60	-1.16	5.35	-0.46	-3.96	-0.24
1.80	-0.71	3.92	-0.35	-3.41	-0.55
2.00	-0.40	2.78	-0.26	-2.92	-0.79
2.20	-0.19	1.91	-0.19	-2.48	-0.94
2.40	-0.07	1.28	-0.13	-2.09	-1.01
2.60	-0.00	0.83	-0.08	-1.75	-1.01
2.80	0.03	0.53	-0.05	-1.46	-0.96
3.00	0.04	0.33	-0.03	-1.22	-0.88
3.20	0.03	0.20	-0.01	-1.00	-0.78
3.40	0.02	0.12	0.00	-0.83	-0.68
3.60	0.01	0.07	0.01	-0.68	-0.58
3.80	0.00	0.04	0.02	-0.56	-0.50
4.00	-0.00	0.02	0.02	-0.46	-0.42
4.20	-0.01	0.01	0.02	-0.38	-0.35
4.40	-0.02	0.01	0.02	-0.31	-0.29
4.60	-0.02	0.00	0.02	-0.25	-0.25
4.80	-0.02	0.00	0.02	-0.21	-0.21
5.00	-0.02	0.00	0.02	-0.17	-0.17