

Supplementary Information for:

**The effect of confinement on the phase behavior of
propane in nanoporous media: An experimental study
probing capillary condensation, evaporation, and
hysteresis at varying pore sizes and temperatures**

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KEYWORDS: Capillary Condensation; Confined Fluids; Propane; Nanopores; MCM-41

Supporting Information

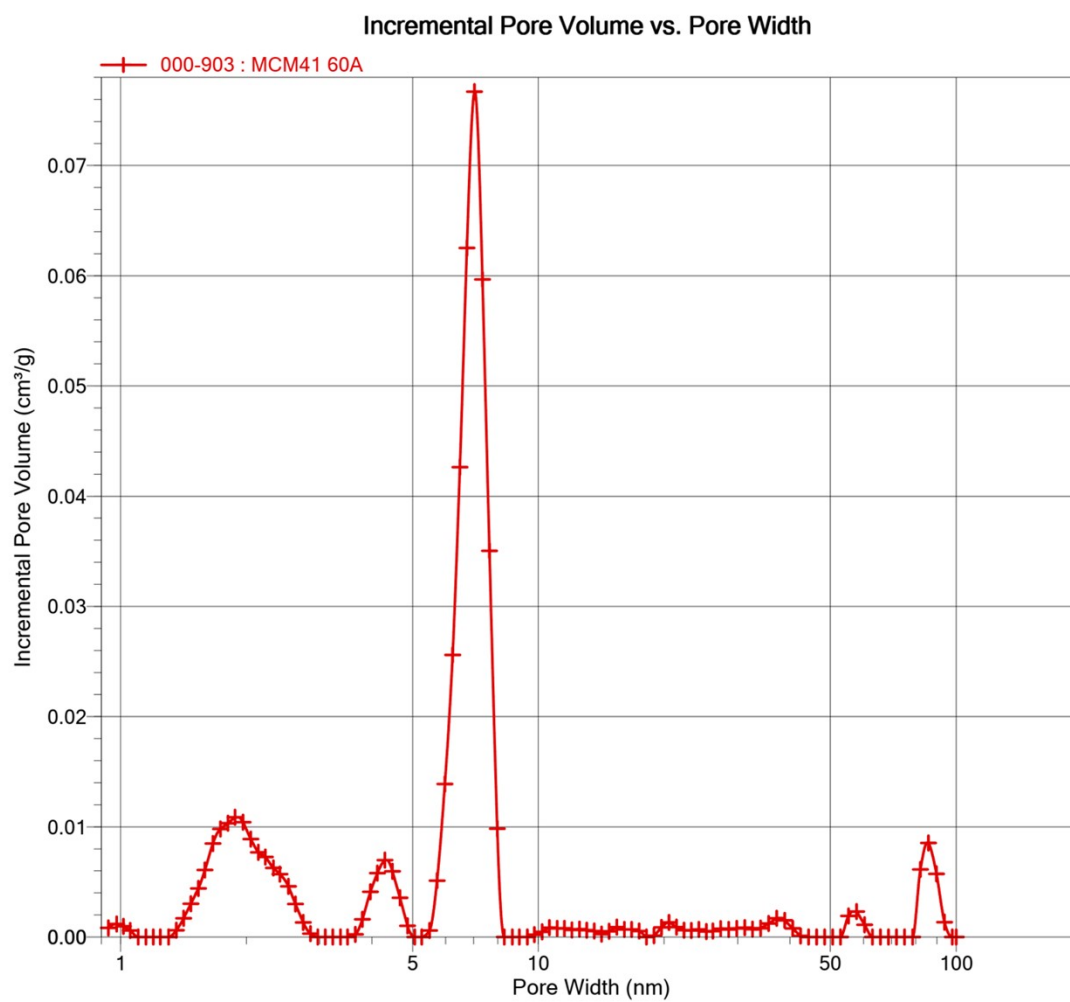


Figure S1. Incremental pore volume vs. pore width for MCM-41 60Å

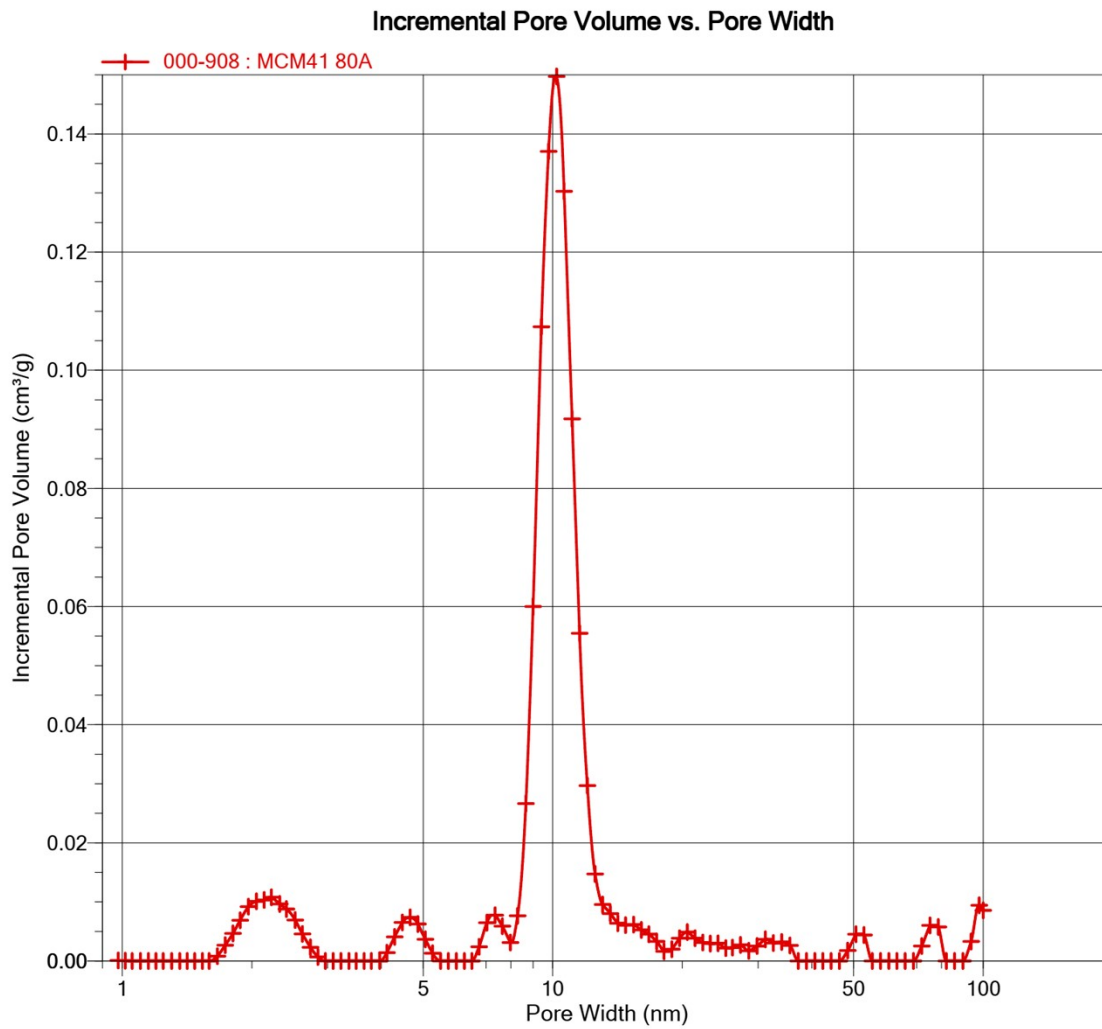


Figure S2. Incremental pore volume vs. pore width for MCM-41 80Å

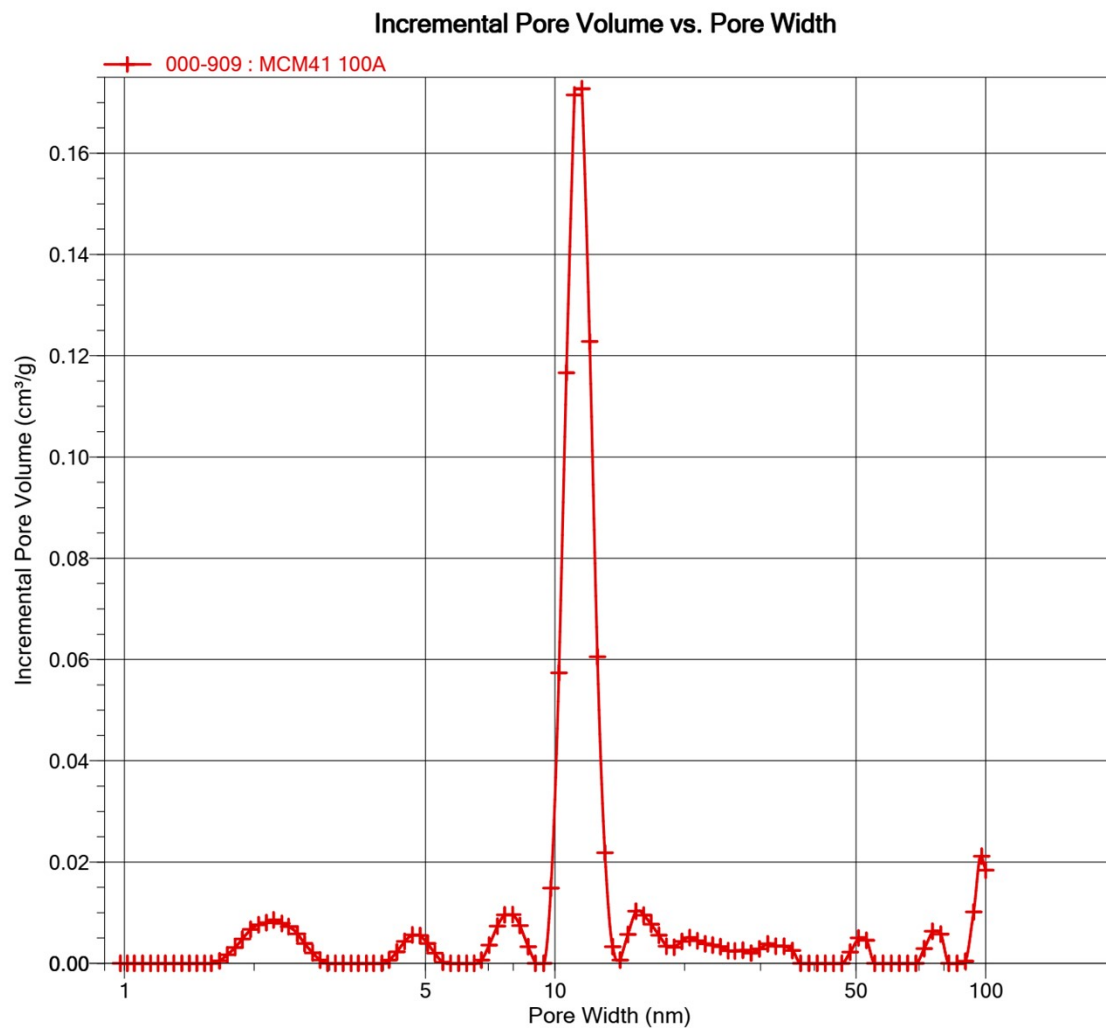


Figure S3. Incremental pore volume vs. pore width for MCM-41 100Å

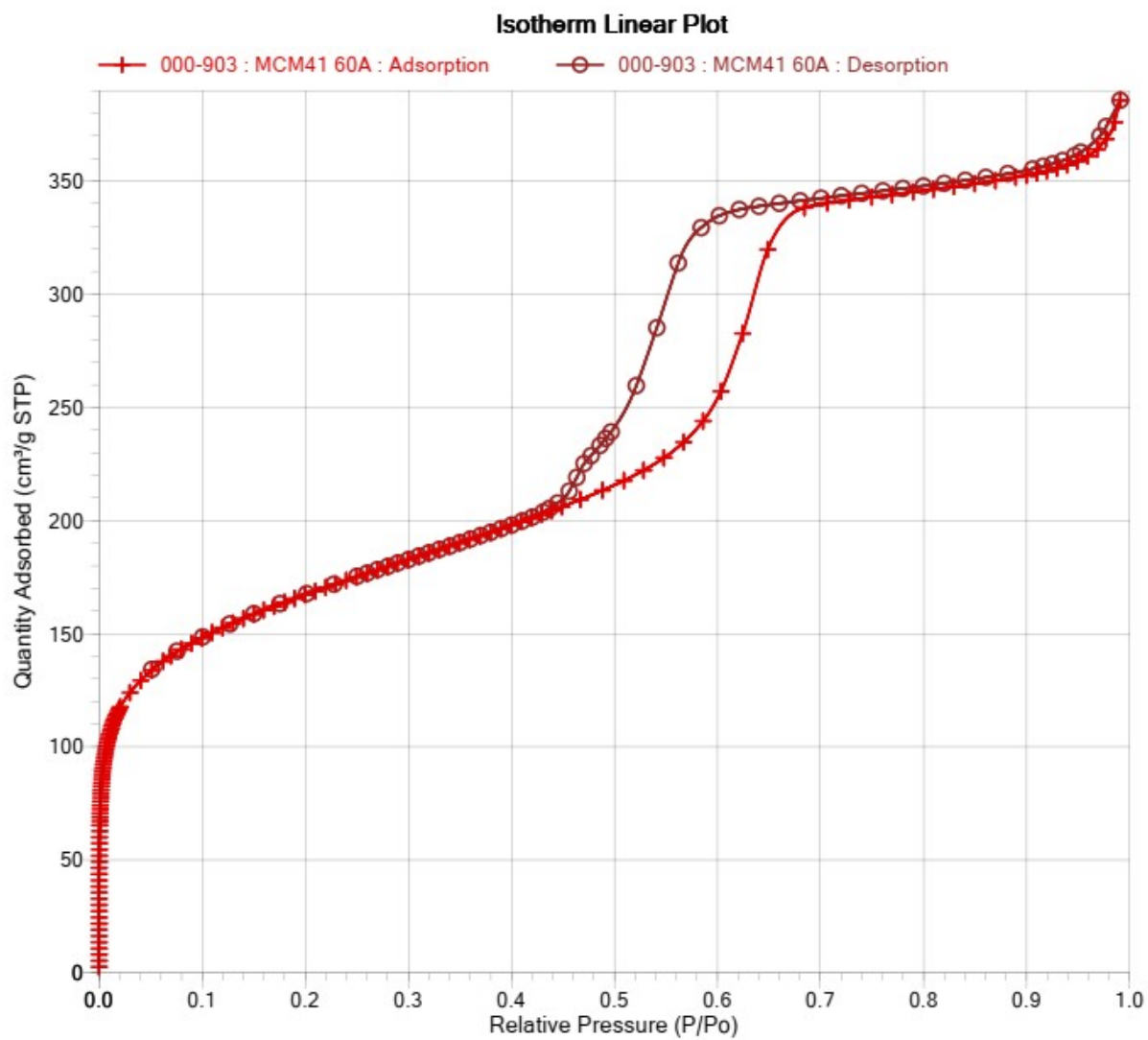


Figure S4. Isotherm Linear Plot for MCM-41 60Å showing Quantity Adsorbed (cm³/g STP) vs Relative Pressure (P/P₀)

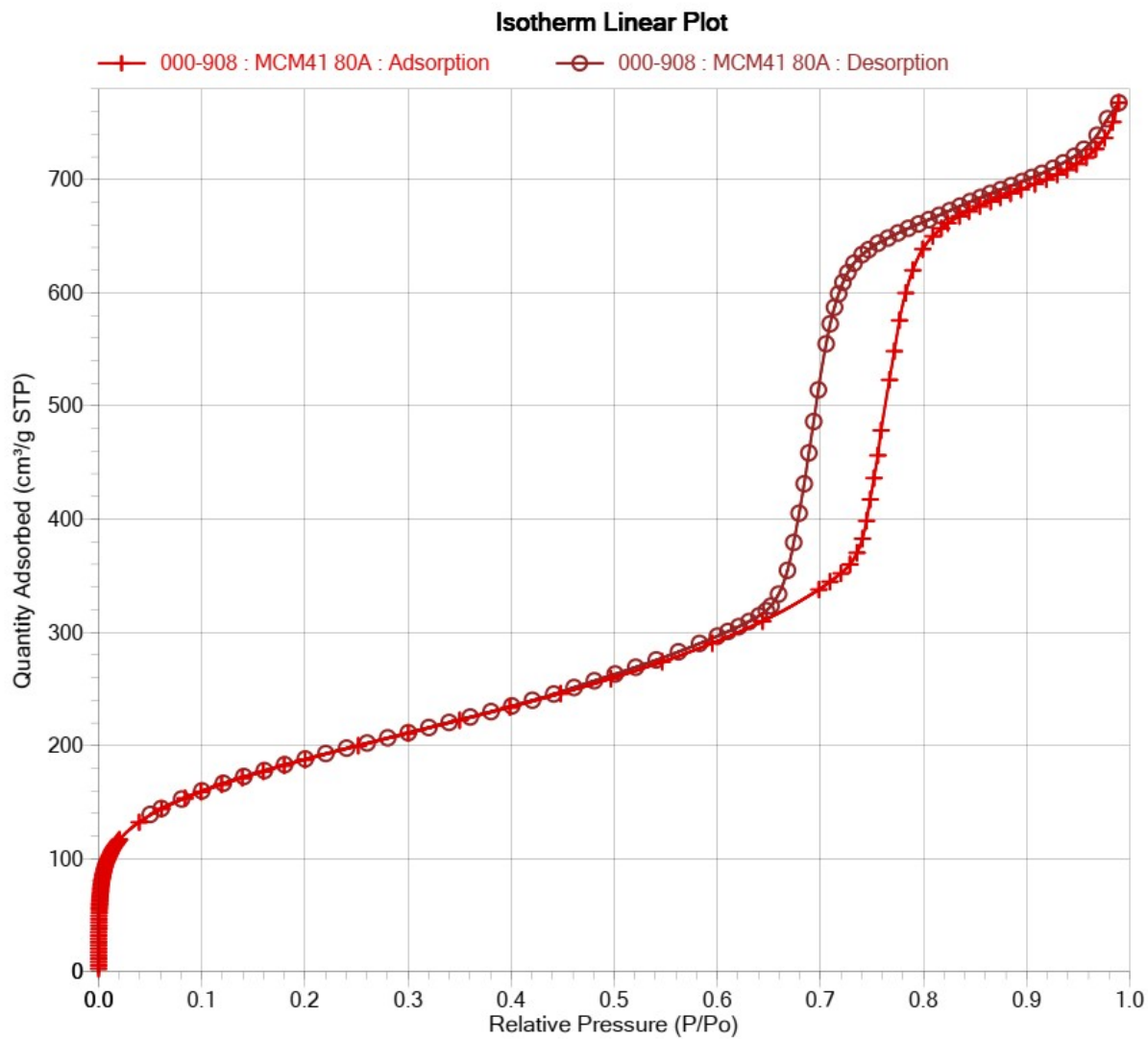


Figure S5. Isotherm Linear Plot for MCM-41 80Å showing Quantity Adsorbed (cm³/g STP) vs Relative Pressure (P/Po)

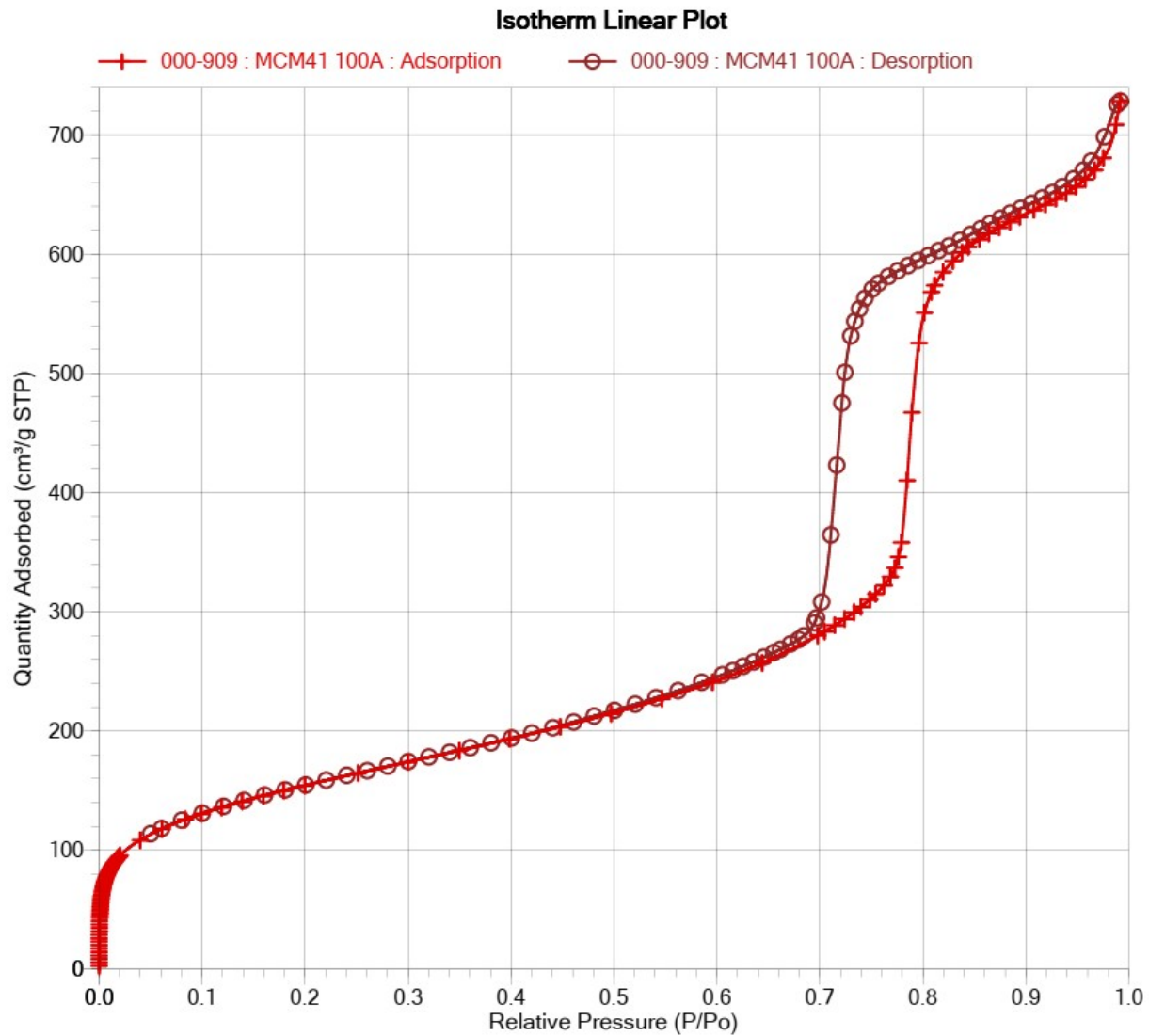


Figure S6. Isotherm Linear Plot for MCM-41 100Å showing Quantity Adsorbed (cm³/g STP) vs Relative Pressure (P/Po)

Table S1. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at -27°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.127	0.000	0.066	0.000	0.112	0.000
0.150	0.233	0.187	0.231	0.211	0.197
0.207	0.473	0.445	0.473	0.409	0.331
0.335	0.696	0.734	0.704	0.656	0.504
0.537	0.931	1.018	0.929	0.896	0.690
0.786	1.151	1.234	1.174	1.123	0.869
1.001	1.375	1.350	1.367	1.291	1.045
1.135	1.594	1.377	1.632	1.389	1.208
1.206	2.070	1.411	2.110	1.434	1.379
1.238	2.302	1.431	2.332	1.462	1.574
1.458	2.525	1.468	2.580	1.467	1.735
1.872	2.738	1.623	2.808	1.471	1.931
1.910	2.885	1.826	3.042	1.488	2.304
1.922	2.973	1.854	3.115	1.533	2.451
		1.864	3.146	1.655	2.647
		1.868	3.187	1.804	2.817
		1.876	3.256	1.873	3.007
		1.885	3.340	1.895	3.171
				1.908	3.325

Table S2. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at -27°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
1.792	3.013	1.771	3.271	1.761	3.065
1.784	2.938	1.761	3.250	1.761	3.017
1.749	2.763	1.757	3.196	1.748	2.965
1.719	2.705	1.742	3.128	1.745	2.918
1.658	2.651	1.725	3.050	1.726	2.859
1.557	2.594	1.668	2.984	1.677	2.776
1.442	2.547	1.588	2.888	1.607	2.694

1.321	2.514	1.508	2.832	1.539	2.609
1.206	2.470	1.447	2.736	1.481	2.533
1.127	2.444	1.384	2.672	1.419	2.472
1.099	2.415	1.332	2.594	1.371	2.386
1.072	2.369	1.298	2.468	1.346	2.322
1.060	2.337	1.269	2.275	1.328	2.264
1.045	2.272	1.263	2.215	1.304	2.052
1.031	2.172	1.252	2.106	1.288	1.724
1.007	1.978	1.246	2.047	1.286	1.461
1.001	1.908	1.236	1.847	1.280	1.271
0.995	1.851	1.231	1.726	1.271	1.150
0.977	1.661	1.224	1.646	1.253	1.079
0.972	1.596	1.214	1.454	1.218	1.027
0.961	1.507	1.196	1.274	1.170	0.969
0.930	1.416	1.186	1.234	1.117	0.908
0.909	1.390	1.165	1.178	1.067	0.852
0.892	1.363	1.128	1.090	1.015	0.803
0.829	1.281	1.042	0.988	0.964	0.752
0.802	1.255	1.000	0.961	0.902	0.712
0.779	1.234	0.906	0.873	0.854	0.665
0.704	1.169	0.865	0.837	0.799	0.634
0.627	1.090	0.779	0.769	0.753	0.605
0.586	1.053	0.695	0.693	0.704	0.565
0.550	1.024	0.649	0.656	0.657	0.535
0.459	0.939	0.618	0.638	0.619	0.507
0.435	0.910	0.443	0.507	0.582	0.480
0.387	0.867	0.366	0.419	0.540	0.450
0.354	0.829	0.287	0.364	0.499	0.441
0.318	0.798	0.236	0.323	0.478	0.412
0.270	0.741	0.203	0.302	0.447	0.394
0.238	0.698	0.182	0.281	0.417	0.380
0.204	0.654	0.168	0.265	0.390	0.359
0.159	0.598	0.151	0.249	0.368	0.349
		0.151	0.239	0.351	0.321
		0.136	0.231	0.331	0.314

				0.287	0.277
				0.247	0.260
				0.230	0.232
				0.202	0.224
				0.185	0.201
				0.167	0.178
				0.151	0.175
				0.146	0.165
				0.133	0.152
				0.121	0.147
				0.115	0.141

Table S3. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at -21°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.128	0.000	0.066	0.000	0.112	0.000
0.152	0.227	0.216	0.221	0.242	0.170
0.157	0.228	0.498	0.456	0.480	0.350
0.237	0.461	0.854	0.678	0.479	0.354
0.408	0.699	0.852	0.688	0.770	0.522
0.657	0.918	1.191	0.896	1.063	0.674
0.957	1.143	1.471	1.116	1.330	0.824
1.227	1.355	1.657	1.351	1.537	1.001
1.396	1.573	1.711	1.577	1.703	1.151
1.463	1.800	1.725	1.799	1.704	1.173
1.506	2.026	1.749	2.046	1.772	1.338
1.537	2.246	1.768	2.254	1.812	1.507
1.640	2.468	1.801	2.477	1.821	1.675
2.208	2.653	1.902	2.714	1.836	1.870
2.357	2.865	2.143	2.936	1.838	2.044
2.379	3.016	2.311	3.133	1.851	2.196
2.379	3.089	2.307	3.121	1.865	2.383
2.382	3.140	2.314	3.189	1.962	2.557
2.382	3.182	2.325	3.219	1.963	2.552

2.386	3.186	2.325	3.303	2.131	2.713
		2.335	3.387	2.120	2.703
		2.339	3.500	2.274	2.870
		2.343	3.597	2.332	3.035
				2.350	3.216
				2.366	3.379
				2.367	3.607

Table S4. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at -21°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
2.241	3.192	2.237	3.206	2.185	2.992
2.230	3.033	2.251	3.231	2.105	2.867
2.213	2.877	2.253	3.235	1.963	2.700
2.149	2.728	2.249	3.228	1.829	2.556
1.895	2.600	2.238	3.192	1.725	2.444
1.542	2.490	2.188	3.046	1.675	2.320
1.395	2.394	2.040	2.898	1.658	2.213
1.361	2.310	2.038	2.902	1.642	1.980
1.346	2.221	1.872	2.761	1.640	1.861
1.328	2.133	1.751	2.642	1.628	1.747
1.307	1.961	1.694	2.525	1.625	1.527
1.292	1.878	1.663	2.414	1.613	1.436
1.285	1.793	1.648	2.305	1.605	1.318
1.273	1.705	1.630	2.185	1.589	1.197
1.246	1.537	1.626	2.080	1.506	1.089
1.213	1.459	1.613	1.968	1.403	0.992
1.136	1.387	1.612	1.848	1.293	0.906
1.063	1.315	1.596	1.739	1.187	0.828
0.979	1.246	1.591	1.628	1.067	0.757
0.907	1.190	1.584	1.516	0.964	0.692
0.831	1.134	1.572	1.407	0.863	0.639
0.764	1.085	1.549	1.312	0.770	0.593
0.762	1.085	1.496	1.205	0.691	0.538

0.712	1.040	1.496	1.219	0.615	0.492
0.658	0.998	1.405	1.122	0.559	0.458
0.608	0.966	1.308	1.036	0.502	0.425
0.563	0.928	1.208	0.945	0.450	0.397
0.517	0.898	1.103	0.878	0.414	0.375
0.483	0.875	1.003	0.790	0.377	0.354
0.450	0.840	0.910	0.743	0.348	0.326
0.428	0.825	0.827	0.679	0.317	0.304
0.403	0.806	0.746	0.646	0.298	0.323
0.327	0.728	0.679	0.609	0.283	0.289
0.323	0.727	0.614	0.571	0.256	0.265
0.279	0.674	0.558	0.519	0.239	0.256
0.238	0.630	0.510	0.505	0.225	0.255
0.237	0.637	0.475	0.473	0.216	0.254
0.204	0.593	0.430	0.447	0.201	0.224
0.187	0.558	0.403	0.422	0.184	0.223
0.170	0.536	0.372	0.389	0.182	0.211
0.154	0.524	0.344	0.394	0.167	0.206
0.139	0.491	0.318	0.370	0.165	0.209
0.126	0.480	0.296	0.361	0.152	0.199
0.125	0.462	0.279	0.339	0.152	0.190
0.109	0.447	0.262	0.329	0.144	0.194
0.107	0.437	0.246	0.298	0.137	0.178
0.099	0.425	0.229	0.300	0.130	0.168
0.092	0.396	0.222	0.291	0.125	0.173
0.080	0.386	0.102	0.207	0.119	0.181
0.078	0.365	0.089	0.214	0.118	0.164
0.073	0.360			0.109	0.154
0.067	0.357			0.093	0.149
				0.036	0.082

Table S5. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at -15°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)

0.138	0.000	0.066	0.000	0.114	0.000
0.321	0.528	0.715	0.513	0.691	0.414
0.989	1.049	1.631	1.024	1.502	0.798
1.320	1.252	2.095	1.549	1.775	0.966
1.599	1.452	2.134	1.781	1.999	1.113
1.766	1.660	2.158	1.965	2.151	1.270
1.832	1.872	2.181	2.182	2.217	1.446
1.869	2.088	2.213	2.413	2.244	1.587
1.904	2.298	2.280	2.642	2.257	1.749
2.125	2.505	2.499	2.835	2.266	1.907
2.720	2.678	2.765	3.024	2.286	2.223
2.882	2.873	2.853	3.212	2.313	2.397
2.915	3.068	2.861	3.244	2.423	2.548
2.919	3.218	2.880	3.394	2.593	2.708
2.921	3.299	2.881	3.436	2.769	2.861
2.927	3.380	2.882	3.508	2.850	3.015
		2.889	3.582	2.883	3.163
		2.893	3.674	2.899	3.321

Table S6. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at -15°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
2.783	3.328	2.814	3.926	2.711	2.989
2.756	3.047	2.797	3.665	2.456	2.726
2.674	2.774	2.796	3.494	2.187	2.476
2.056	2.540	2.769	3.272	2.098	2.250
1.735	2.370	2.577	2.986	2.076	2.038
1.686	2.201	2.236	2.713	2.056	1.804
1.670	2.050	2.103	2.499	2.048	1.610
1.661	1.884	2.062	2.288	2.032	1.400
1.634	1.722	2.040	2.069	1.960	1.171
1.572	1.567	2.017	1.857	1.717	0.990
1.401	1.408	2.000	1.644	1.460	0.835
1.198	1.265	1.959	1.394	1.171	0.676

1.014	1.146	1.773	1.187	0.929	0.558
0.850	1.049	1.511	1.009	0.732	0.468
0.720	0.971	1.240	0.834	0.583	0.409
0.619	0.900	1.007	0.717	0.482	0.356
0.540	0.850	0.805	0.607	0.402	0.324
0.470	0.793	0.659	0.531	0.337	0.277
0.419	0.756	0.548	0.469	0.178	0.181
0.377	0.717	0.454	0.423	0.107	0.137
0.330	0.689	0.388	0.382	0.072	0.100
0.303	0.659	0.331	0.342	0.058	0.092
0.219	0.577	0.295	0.317		
0.146	0.494	0.140	0.160		
0.144	0.485	0.079	0.102		
0.099	0.407				

Table S7. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at -12°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(psia)	(g)	(psia)	(g)	(psia)	(g)
0.134	0.000	0.066	0.000	0.111	0.000
0.240	0.377	0.497	0.392	0.497	0.307
0.586	0.745	1.197	0.729	1.114	0.578
1.150	1.075	1.851	1.049	1.704	0.839
1.724	1.424	2.278	1.415	2.171	1.102
2.008	1.769	2.362	1.795	2.419	1.371
2.086	2.122	2.402	2.145	2.487	1.655
2.227	2.474	2.459	2.498	2.511	1.948
3.125	2.777	2.754	2.870	2.533	2.219
3.224	3.096	3.137	3.169	2.598	2.486
3.228	3.341	3.159	3.338	2.901	2.737
3.234	3.408	3.174	3.475	3.150	2.997
3.250	4.360	3.188	3.755	3.193	3.270
		3.189	3.985	3.216	3.537
		3.203	4.263	3.224	3.689
		3.201	4.689	3.224	4.140

		3.212	4.979	3.225	4.227
		3.218	5.647		

Table S8. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at -12°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(psia)	(g)	(psia)	(g)	(psia)	(g)
3.121	4.738	3.150	6.043	3.117	4.338
3.109	4.643	3.109	4.046	3.125	4.349
3.113	4.473	3.100	3.805	3.112	4.268
3.107	4.427	3.099	3.638	3.110	4.141
3.107	4.348	3.074	3.289	3.091	3.793
3.100	4.205	2.923	3.011	3.062	3.433
3.086	3.857	2.564	2.798	3.031	3.092
3.076	3.325	2.365	2.567	2.786	2.768
2.996	2.799	2.301	2.367	2.504	2.555
1.979	2.402	2.279	2.148	2.371	2.361
1.912	2.242	2.262	1.976	2.334	2.152
1.892	2.089	2.242	1.769	2.307	1.968
1.879	1.931	2.212	1.570	2.293	1.791
1.850	1.779	2.176	1.395	2.286	1.591
1.805	1.622	2.008	1.209	2.274	1.400
1.682	1.483	1.789	1.058	2.222	1.232
1.497	1.370	1.553	0.908	2.008	1.077
1.327	1.248	1.324	0.814	1.781	0.942
1.149	1.156	1.120	0.699	1.537	0.804
1.005	1.077	0.959	0.624	1.308	0.706
0.879	1.012	0.817	0.555	1.105	0.616
0.771	0.941	0.701	0.502	0.936	0.557
0.686	0.887	0.605	0.447	0.800	0.480
0.612	0.843	0.522	0.433	0.674	0.420
0.546	0.804	0.462	0.375	0.582	0.380
0.492	0.759	0.411	0.379	0.504	0.346
0.460	0.728	0.366	0.328	0.438	0.303
0.412	0.702	0.324	0.298	0.389	0.291

0.374	0.672	0.294	0.281	0.341	0.266
0.350	0.649	0.267	0.283	0.309	0.253
0.318	0.630	0.217	0.248	0.273	0.221
0.301	0.608	0.190	0.224	0.256	0.238
0.279	0.593	0.160	0.219	0.236	0.205
0.263	0.574	0.138	0.199	0.216	0.208
0.247	0.560	0.124	0.199	0.201	0.179
0.218	0.536			0.171	0.162
0.200	0.518			0.145	0.153
0.186	0.490			0.128	0.136
0.168	0.469			0.120	0.129
0.159	0.462				
0.146	0.442				

Table S9. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at -9°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.124	0.000	0.066	0.000	0.114	0.000
0.255	0.356	0.519	0.336	0.545	0.290
0.636	0.719	1.246	0.708	1.199	0.536
1.224	1.047	1.946	1.011	1.831	0.794
1.834	1.359	2.461	1.348	2.334	1.054
2.204	1.694	2.612	1.693	2.655	1.304
2.300	2.019	2.645	2.033	2.744	1.567
2.379	2.351	2.703	2.362	2.773	1.825
3.180	2.643	2.848	2.726	2.791	2.099
3.517	2.855	3.342	3.025	2.825	2.350
3.554	3.081	3.488	3.342	3.033	2.614
3.573	3.262	3.500	3.373	3.289	2.796
		3.506	3.452	3.462	2.941
		3.516	3.639	3.513	3.143
		3.534	3.915	3.529	3.339
				3.547	3.519

Table S10. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at -9°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
3.444	3.335	3.467	4.027	3.434	3.709
3.420	3.141	3.434	3.593	3.426	3.588
3.404	3.003	3.424	3.500	3.410	3.455
3.378	2.874	3.401	3.322	3.400	3.332
3.285	2.751	3.351	3.179	3.385	3.213
3.028	2.645	3.183	2.997	3.358	3.078
2.655	2.550	2.943	2.852	3.323	2.956
2.340	2.477	2.739	2.734	3.206	2.846
2.214	2.373	2.634	2.604	3.044	2.706
2.172	2.276	2.588	2.493	2.857	2.586
2.160	2.179	2.562	2.355	2.695	2.456
2.146	1.985	2.551	2.235	2.625	2.331
2.130	1.888	2.529	2.057	2.604	2.217
2.114	1.805	2.509	1.897	2.585	2.086
2.083	1.710	2.493	1.742	2.572	1.966
2.034	1.614	2.470	1.583	2.555	1.711
1.957	1.520	2.432	1.406	2.544	1.587
1.855	1.448	2.293	1.252	2.539	1.471
1.743	1.375	2.108	1.123	2.521	1.353
1.623	1.309	1.634	0.878	2.456	1.218
1.523	1.260	1.397	0.778	2.316	1.114
1.393	1.188	1.213	0.717	2.164	1.024
1.286	1.124	0.979	0.611	2.007	0.933
1.191	1.076	0.867	0.550	1.840	0.862
1.108	1.038	0.615	0.419	1.633	0.758
1.042	1.000	0.529	0.374	1.447	0.694
0.989	0.976	0.173	0.194	1.281	0.627
0.945	0.946			1.053	0.547
0.908	0.933			0.979	0.514
0.875	0.918			0.911	0.475
0.791	0.870			0.877	0.461

0.714	0.832			0.843	0.452
0.651	0.786			0.681	0.372
0.576	0.738			0.573	0.325
0.526	0.703			0.366	0.232
0.470	0.673			0.235	0.168
0.430	0.647			0.187	0.148
0.402	0.618				
0.297	0.528				
0.262	0.501				

Table S11. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at -6°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.128	0.000	0.066	0.000	0.114	0.000
0.329	0.464	0.761	0.440	0.813	0.390
0.977	0.902	1.797	0.878	1.780	0.744
1.829	1.324	2.615	1.321	2.559	1.089
2.434	1.734	2.888	1.741	2.969	1.411
2.529	1.920	2.950	2.168	3.055	1.763
2.540	2.120	3.055	2.611	3.076	2.116
2.559	2.357	3.651	3.027	3.141	2.471
2.973	2.558	3.851	3.300	3.569	2.778
3.873	2.924	3.865	3.524	3.861	3.097
3.917	3.206	3.870	3.748	3.897	3.430
3.915	3.338	3.888	4.007		
3.923	3.424	3.884	4.166		
3.923	3.713	3.899	4.525		
3.929	3.788				

Table S12. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at -6°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
3.808	4.061	3.835	4.839	3.796	3.713
3.798	3.931	3.833	4.658	3.762	3.460

3.789	3.852	3.828	4.647	3.732	3.190
3.783	3.511	3.816	4.441	3.625	2.919
3.760	3.238	3.809	4.240	3.270	2.698
3.724	2.975	3.796	4.021	3.263	2.694
3.726	2.978	3.792	3.836	3.266	2.689
3.472	2.723	3.794	3.816	3.265	2.691
2.691	2.536	3.784	3.685	2.985	2.480
2.436	2.380	3.765	3.407	2.900	2.273
2.405	2.209	3.682	3.159	2.874	2.071
2.388	2.047	3.324	2.915	2.868	2.067
2.399	2.044	2.996	2.683	2.851	1.872
2.359	1.881	2.876	2.493	2.835	1.680
2.298	1.733	2.828	2.305	2.820	1.465
2.174	1.583	2.809	2.089	2.732	1.281
1.976	1.453	2.786	1.893	2.476	1.103
1.756	1.336	2.756	1.689	2.169	0.961
1.542	1.232	2.720	1.506	2.175	0.959
1.353	1.141	2.572	1.321	2.173	0.949
1.191	1.064	2.323	1.177	1.877	0.826
1.053	0.994	2.051	1.048	1.604	0.726
0.938	0.927	1.787	0.915	1.357	0.646
0.826	0.882	1.542	0.810	1.149	0.542
0.741	0.840	1.323	0.743	0.973	0.489
0.669	0.797	1.140	0.639	0.830	0.437
0.603	0.758	0.974	0.552	0.832	0.434
0.543	0.728	0.848	0.511	0.714	0.398
0.546	0.727	0.854	0.515	0.615	0.359
0.504	0.695	0.735	0.469	0.532	0.322
0.459	0.673	0.649	0.429	0.465	0.297
0.423	0.645	0.655	0.433	0.414	0.261
0.390	0.624	0.572	0.397	0.365	0.248
0.391	0.627	0.505	0.361	0.332	0.228
0.371	0.599	0.453	0.344	0.296	0.219
0.339	0.582	0.454	0.341	0.267	0.196
0.325	0.569	0.396	0.299	0.249	0.200

0.308	0.552	0.365	0.301	0.230	0.177
0.289	0.538	0.323	0.274	0.227	0.174
0.287	0.537	0.302	0.277	0.226	0.190
0.274	0.533	0.276	0.264	0.236	0.177
0.256	0.514	0.255	0.236	0.230	0.171
0.247	0.504	0.236	0.231	0.214	0.177
0.237	0.488	0.222	0.221	0.209	0.160
0.224	0.480	0.209	0.212	0.215	0.174
0.215	0.475	0.193	0.198	0.200	0.164
0.211	0.461	0.193	0.192	0.184	0.146
0.195	0.453	0.182	0.204	0.168	0.136
0.189	0.444	0.181	0.196	0.161	0.142
0.178	0.439	0.169	0.204	0.153	0.146
0.173	0.417	0.164	0.188	0.138	0.126
0.170	0.422	0.153	0.191	0.137	0.142
0.170	0.417	0.146	0.179	0.130	0.128
0.162	0.400	0.146	0.166	0.134	0.124
0.159	0.397	0.148	0.171	0.126	0.123
0.149	0.394	0.142	0.174	0.117	0.119
		0.129	0.165	0.109	0.119
		0.127	0.165	0.115	0.122
		0.126	0.173	0.112	0.110
		0.125	0.155	0.101	0.112
		0.126	0.164	0.102	0.114
		0.110	0.146	0.102	0.113
		0.108	0.160	0.093	0.105
		0.10762	0.153	0.08631	0.103

Table S13. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at -3°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.133	0.000	0.066	0.000	0.119	0.000
0.220	0.280	0.428	0.291	0.467	0.220
0.481	0.546	0.990	0.518	1.003	0.425

0.890	0.805	1.606	0.752	1.561	0.612
0.890	0.806	2.169	0.990	1.564	0.605
1.405	1.041	2.633	1.186	2.104	0.799
1.922	1.264	2.994	1.381	2.565	0.981
2.364	1.476	3.167	1.608	2.927	1.160
2.661	1.690	3.205	1.815	3.199	1.322
2.786	1.913	3.238	2.060	3.318	1.499
2.839	2.120	3.272	2.284	3.356	1.678
2.902	2.343	3.321	2.482	3.375	1.845
3.179	2.538	3.421	2.677	3.389	2.019
3.902	2.696	3.712	2.871	3.406	2.191
3.900	2.695	4.060	3.076	3.437	2.351
4.229	2.871	4.212	3.249	3.507	2.518
4.279	3.056	4.227	3.312	3.732	2.662
4.306	3.176	4.229	3.312	3.972	2.812
4.306	3.254			4.165	2.965
4.310	3.304			4.246	3.108
4.312	3.313			4.268	3.250

Table S14. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at -3°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
4.177	3.344	4.171	3.428	4.157	3.400
4.171	3.306	4.177	3.428	4.104	3.158
4.148	3.155	4.164	3.390	3.948	2.911
4.092	2.909	4.102	3.240	3.588	2.688
3.671	2.687	3.794	3.000	3.305	2.493
2.915	2.520	3.802	2.991	3.221	2.308
2.733	2.358	3.418	2.804	3.190	2.097
2.699	2.200	3.222	2.598	3.175	1.922
2.668	2.046	3.165	2.408	3.158	1.729
2.635	1.894	3.132	2.226	3.130	1.544

2.568	1.744	3.106	2.047	3.070	1.356
2.440	1.598	3.081	1.869	2.822	1.174
2.244	1.477	3.042	1.722	2.532	1.033
2.002	1.367	2.995	1.525	2.226	0.886
1.783	1.257	2.823	1.331		
		2.565	1.199		

Table S15. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at 0°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.131	0.000	0.066	0.000	0.107	0.000
0.277	0.334	0.070	0.015	0.646	0.290
0.671	0.659	0.572	0.334	0.639	0.286
1.292	0.951	0.570	0.321	0.638	0.278
1.963	1.236	1.355	0.623	1.407	0.539
2.565	1.493	1.359	0.610	2.155	0.773
2.951	1.737	2.149	0.874	3.141	1.146
3.101	1.975	2.802	1.172	3.511	1.362
3.174	2.237	3.276	1.419	3.507	1.370
3.261	2.464	3.500	1.677	3.662	1.570
3.969	2.660	3.552	1.914	3.698	1.783
4.570	2.840	3.586	2.166	3.703	1.793
4.692	3.030	3.635	2.422	3.699	1.784
4.723	3.182	3.712	2.675	3.731	1.969
4.727	3.216	3.997	2.882	3.749	2.187
4.726	3.288	4.410	3.090	3.783	2.386
4.733	3.320	4.619	3.265	3.906	2.575
4.733	3.432	4.645	3.321	3.905	2.579
4.739	3.458	4.650	3.368	4.180	2.746
4.742	3.492	4.665	3.470	4.468	2.901
		4.677	3.592	4.628	3.065
		4.682	3.657	4.680	3.231
		4.701	3.824	4.679	3.220
		4.701	3.947	4.710	3.370

		4.706	4.072	4.721	3.472
		4.711	4.240	4.727	3.535
		4.717	4.422	4.722	3.579
		4.722	4.705	4.730	3.617
				4.733	3.672
				4.731	3.696

Table S16. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at 0°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
4.605	3.461	4.656	4.722	4.619	3.778
4.604	3.444	4.635	4.589	4.607	3.725
4.592	3.394	4.627	4.426	4.572	3.451
4.574	3.226	4.615	4.250	4.464	3.054
4.522	2.993	4.601	4.107	3.892	2.687
4.232	2.767	4.588	3.851	3.585	2.347
3.464	2.592	4.569	3.593	3.530	2.039
3.065	2.435	4.534	3.336	3.499	1.708
3.022	2.284	4.402	3.101	3.430	1.412
2.997	2.131	3.993	2.878	2.966	1.147
2.945	1.985	3.657	2.704	2.416	0.896
2.878	1.823	3.524	2.498	1.902	0.748
2.765	1.685	3.473	2.332	1.495	0.603
2.573	1.558	3.450	2.162	1.171	0.499
2.348	1.438	3.423	1.964	0.924	0.431
2.111	1.338	3.396	1.772	0.743	0.376
1.885	1.246	3.364	1.610	0.608	0.318
1.684	1.158	3.279	1.452	0.421	0.244
1.489	1.087	3.033	1.264	0.179	0.128
1.346	1.026	2.758	1.130	0.057	0.065
1.207	0.970	2.466	1.037		
1.088	0.919	2.181	0.941		
0.990	0.876	1.924	0.845		
0.898	0.830	1.689	0.759		

0.817	0.799	1.485	0.661		
0.747	0.765	1.310	0.601		
0.687	0.733	1.016	0.513		
0.639	0.707	0.905	0.456		
0.550	0.651	0.801	0.415		
0.504	0.632	0.716	0.399		
0.473	0.613	0.652	0.375		
0.392	0.568	0.521	0.312		
0.335	0.523	0.474	0.301		
0.222	0.430	0.435	0.289		
0.172	0.371	0.397	0.264		
0.133	0.314	0.365	0.258		
		0.346	0.239		
		0.263	0.199		
		0.176	0.138		
		0.147	0.100		
		0.128	0.096		
		0.070	0.055		

Table S17. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at +3°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.135	0.000	0.066	0.000	0.110	0.000
0.292	0.334	0.622	0.375	0.690	0.280
0.730	0.659	1.469	0.686	1.521	0.533
1.384	0.975	2.301	0.958	2.331	0.780
2.126	1.240	3.001	1.222	3.024	1.005
2.754	1.478	3.523	1.464	3.541	1.212
3.208	1.720	3.832	1.698	3.894	1.405
3.396	1.947	3.900	1.911	4.037	1.607
3.483	2.176	3.935	2.125	4.084	1.779
3.560	2.394	3.982	2.321	4.101	1.967
3.896	2.596	4.023	2.516	4.116	2.139
4.622	2.742	4.102	2.710	4.138	2.331
5.014	2.866	4.304	2.898	4.202	2.503
5.130	2.987	4.639	3.035	4.397	2.645
5.166	3.139	4.924	3.193	4.643	2.777
5.186	3.236	5.056	3.315	4.878	2.900
5.205	3.342	5.089	3.353	5.033	3.023
		5.084	3.367	5.108	3.142
		5.124	3.462	5.141	3.244
		5.149	3.654	5.158	3.321
		5.165	3.778	5.169	3.377
		5.173	3.820	5.180	3.487
		5.174	3.918		

Table S18. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at +3°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
		5.121	4.052	5.071	3.501
		5.089	3.918	5.059	3.468

		5.056	3.716	5.040	3.410
		5.007	3.468	5.046	3.413
		4.723	3.132	4.933	3.088
		4.114	2.849	4.452	2.782
		3.883	2.583	4.019	2.527
		3.813	2.323	4.019	2.523
		3.772	2.061	3.917	2.255
		3.721	1.797	3.883	2.005
		3.602	1.563	3.858	1.708
		3.188	1.325	3.757	1.428
		2.729	1.141	3.328	1.202
		2.285	0.987	2.815	0.997
		1.894	0.837	2.325	0.829
		1.568	0.726	1.894	0.692
		1.574	0.736	1.536	0.596
		1.572	0.733	1.252	0.507
		1.299	0.629	1.032	0.443
		1.085	0.580	0.849	0.392
		0.912	0.515	0.715	0.338
		0.907	0.513	0.597	0.296
		0.919	0.507	0.515	0.269
		0.782	0.459	0.447	0.254
		0.782	0.469	0.382	0.222
		0.665	0.403	0.335	0.199
		0.569	0.356	0.298	0.186
		0.487	0.329	0.270	0.181
		0.436	0.322	0.267	0.186
		0.384	0.295	0.249	0.154
		0.390	0.288	0.224	0.150
		0.347	0.283	0.218	0.149
		0.309	0.263	0.202	0.150
		0.273	0.259	0.188	0.150
		0.249	0.233	0.186	0.144
		0.227	0.224	0.173	0.133
		0.212	0.202	0.166	0.127

		0.204	0.194	0.151	0.125
		0.185	0.194	0.137	0.116
		0.172	0.194	0.137	0.100
		0.157	0.189	0.120	0.106
		0.154	0.169	0.120	0.094
		0.155	0.175	0.120	0.084
		0.140	0.178	0.116	0.097
		0.138	0.169	0.105	0.086
		0.124	0.157	0.104	0.082
		0.127	0.147	0.097	0.081
		0.126	0.167	0.086	0.084
		0.110	0.160	0.083	0.065
		0.096	0.145	0.082	0.067
		0.092	0.150	0.071	0.065
		0.076	0.141	0.070	0.067
		0.077	0.146	0.071	0.063
		0.067	0.130	0.058	0.066
		0.066	0.137	0.055	0.062
		0.060	0.127	0.055	0.049
		0.057	0.114	0.053	0.059
		0.056	0.132	0.052	0.049
		0.053	0.110	0.045	0.045
		0.048	0.122	0.051	0.044
		0.057	0.118	0.047	0.048
		0.057	0.119	0.039	0.045
		0.056	0.124	0.037	0.045
		0.05145	0.117	0.03685	0.047
		0.04168	0.124	0.03665	0.036
		0.04614	0.119	0.03711	0.034
		0.05231	0.124	0.03771	0.026
		0.04903	0.119	0.03093	0.035

Table S19. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at +12°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.000	0.000	0.066	0.000	0.000	0.000
0.149	0.211	0.414	0.085	0.217	0.068
0.480	0.418	0.952	0.205	0.496	0.197
0.951	0.605	1.560	0.357	0.843	0.303
1.566	0.785	2.193	0.545	1.190	0.417
2.172	0.946	2.801	0.786	1.612	0.558
2.773	1.109	3.385	1.011	2.022	0.630
3.339	1.270	3.883	1.249	2.445	0.757
3.824	1.398	4.296	1.378	2.853	0.849
4.194	1.557	4.645	1.575	3.265	0.947
4.405	1.694	4.933	1.737	3.623	1.050
4.520	1.862	5.113	1.987	3.941	1.180
4.604	2.021	5.181	2.106	4.243	1.292
4.707	2.161	5.290	2.378	4.538	1.400
5.119	2.337	5.329	2.453	4.782	1.471
5.767	2.420	5.575	2.799	4.989	1.565
6.297	2.501	5.845	2.994	5.313	1.735
6.566	2.609	6.150	3.088	5.434	1.830
6.641	2.715	6.441	3.123	5.503	1.913
6.667	2.808	6.626	3.216	5.536	2.004
6.684	2.868	6.709	3.345	5.553	2.077
6.711	3.182	6.747	3.355	5.579	2.328
6.718	3.207	6.753	3.454	5.603	2.489
6.722	3.313	6.765	3.490	5.621	2.610
6.726	3.316	6.771	3.612	5.652	2.797
		6.784	3.718	5.751	3.037
				5.878	3.155
				6.067	3.288
				6.252	3.373
				6.431	3.450

				6.606	3.555
				6.731	3.619
				6.749	3.640
				6.769	3.645
				6.788	3.682
				6.797	3.684
				6.797	3.708

Table S20. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at +12°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
6.725	3.367	--	--	6.801	3.715
6.717	3.297	--	--	6.805	3.701
6.682	3.086	--	--	6.774	3.698
6.660	2.957	--	--	6.607	3.603
6.622	2.754	--	--	6.314	3.462
6.542	2.611	--	--	6.041	3.363
6.194	2.465	--	--	5.793	3.243
5.518	2.324	--	--	5.576	3.142
4.949	2.233	--	--	5.454	3.024
4.665	2.114	--	--	5.392	2.897
4.578	1.993	--	--	5.356	2.774
4.516	1.902	--	--	5.327	2.671
4.453	1.788	--	--	5.302	2.552
4.371	1.670	--	--	5.283	2.455
4.254	1.564	--	--	5.263	2.345
4.070	1.453	--	--	5.255	2.219
3.844	1.367	--	--	5.237	2.119
3.592	1.295	--	--	5.218	2.006
3.346	1.225	--	--	5.190	1.873
3.106	1.158	--	--	5.102	1.753
2.877	1.081	--	--	4.944	1.666
2.660	1.054			4.766	1.571
2.462	0.999			4.579	1.477

2.275	0.949			4.376	1.403
2.106	0.907			4.166	1.315
1.811	0.831			3.957	1.266
1.681	0.814			3.748	1.183
1.372	0.707			3.534	1.115
1.071	0.616			3.330	1.064
0.951	0.570			3.136	1.009
0.852	0.538			2.687	0.865
0.697	0.478			2.289	0.755
0.490	0.404			1.945	0.647
0.452	0.393			1.661	0.590
0.419	0.369			1.426	0.514
				1.224	0.463
				1.055	0.391
				0.917	0.359
				0.806	0.330
				0.705	0.289
				0.620	0.280
				0.552	0.255
				0.493	0.225
				0.443	0.199

Table S21. Experimentally measured values of pressure and mass during adsorption of Propane in MCM-41 at +20°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
0.000	0.000	0.066	0.000	0.000	0.000
0.171	0.166	0.478	0.047	0.327	0.152
0.568	0.403	1.075	0.126	0.800	0.286
1.087	0.550	3.095	0.258	1.373	0.457
1.714	0.727	4.310	0.425	1.928	0.579
2.371	0.884	4.808	0.544	2.501	0.712
3.037	1.041	5.235	0.680	3.028	0.838
3.668	1.199	5.598	0.801	3.544	0.955
4.237	1.313	5.929	0.876	4.007	1.080

4.738	1.440	6.179	0.977	4.431	1.173
5.149	1.548	6.380	1.165	4.813	1.286
5.456	1.698	6.462	1.333	5.151	1.383
5.637	1.799	6.664	1.848	5.461	1.492
5.743	1.932	6.732	2.021	5.730	1.590
5.831	2.064	6.790	2.077	5.963	1.656
5.921	2.171	6.886	2.200	6.183	1.743
6.095	2.292	7.039	2.273	6.360	1.839
6.569	2.362	7.227	2.313	6.509	1.917
7.019	2.430	8.128	2.488	6.630	1.985
7.398	2.481	8.195	2.508	6.690	2.093
7.689	2.508	8.238	2.592	6.712	2.169
7.909	2.565	8.270	2.885	6.729	2.247
8.145	2.632			6.736	2.316
8.199	2.688			6.751	2.423
8.230	2.721			6.762	2.492
8.254	2.750			6.772	2.575
8.270	2.774			6.780	2.637
				6.793	2.737
				6.809	2.828
				6.820	2.906
				6.841	2.992
				6.879	3.041
				6.935	3.126
				7.025	3.186
				7.136	3.261
				7.264	3.310
				7.387	3.384
				7.500	3.436
				7.613	3.495
				7.724	3.511
				7.823	3.557
				7.926	3.607
				8.010	3.644
				8.082	3.685

				8.152	3.745
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Table S22. Experimentally measured values of pressure and mass during desorption of Propane in MCM-41 at +20°C.

60 Å		80 Å		100 Å	
Pressure	Mass	Pressure	Mass	Pressure	Mass
(bar)	(g)	(bar)	(g)	(bar)	(g)
8.284	2.857	8.227	2.932	8.208	3.793
7.926	2.603	7.896	2.503	7.814	3.579
6.824	2.424	7.286	2.332	7.338	3.378
5.989	2.253	6.794	2.245	6.932	3.177
5.802	2.050	6.600	1.988	6.764	3.001
5.657	1.854	6.511	1.757	6.706	2.788
5.437	1.698	6.447	1.530	6.669	2.591
5.053	1.543	6.391	1.450	6.639	2.386
4.573	1.391	6.251	1.077	6.603	2.189
4.079	1.287	5.969	0.878	6.554	1.995
3.629	1.189	5.576	0.702	6.290	1.846
3.226	1.090	5.152	0.612	5.939	1.654
2.540	0.980	4.726	0.526	5.543	1.524
2.261	0.882	4.303	0.392	5.130	1.394
2.019	0.815	3.162	0.243	4.716	1.271
1.808	0.761			4.314	1.139
1.623	0.744			3.908	1.035
1.323	0.652			3.544	0.949
1.201	0.618			3.211	0.873
1.094	0.608			2.907	0.807
1.000	0.571			2.630	0.759
0.920	0.551			2.156	0.650
0.847	0.522			1.611	0.516
0.721	0.461			1.029	0.318
				0.736	0.234
				0.680	0.228
				0.582	0.182