

Supporting Information

Unveiling the Temperature Influence on the Sorptive Behavior of ZIF-8 Composite Materials Impregnated with [C_nMIM][B(CN)₄] Ionic Liquids

Tiago J. Ferreira ¹, Laura M. Esteves ¹, José M. S. S. Esperança ^{1,*}, Isabel A. A. C. Esteves ^{1,*}

¹ LAQV/REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, 2829-516, Caparica, Portugal

* Correspondence: jmesp@fct.unl.pt (José M. S. S. Esperança); i.esteves@fct.unl.pt (Isabel A. A. C. Esteves)

S1. Single-component CO₂, CH₄ and N₂ adsorption-desorption data of ZIF-8 and IL@ZIF-8 composites at 303 K

Table S1. CO₂, CH₄ and N₂ adsorption-desorption equilibrium data at 303 K for pristine ZIF-8.

CO ₂ – 303 K		CH ₄ – 303 K		N ₂ – 303 K	
P (bar)	q _{exc} (mol/kg)	P (bar)	q _{exc} (mol/kg)	P (bar)	q _{exc} (mol/kg)
0.057	0.032	0.500	0.116	0.502	0.049
0.315	0.186	0.998	0.238	1.001	0.089
0.808	0.488	3.073	0.706	2.943	0.258
1.572	0.909	5.877	1.294	6.049	0.505
2.596	1.603	8.007	1.694	7.989	0.645
4.492	2.902	11.949	2.319	12.079	0.930
7.11	4.429	15.980	2.821	16.010	1.165
9.55	5.445	14.019	2.586	14.009	1.047
13.699	6.539	10.017	2.023	9.893	0.789
16.141	6.953	4.539	1.026	4.512	0.395
10.577	5.813	1.939	0.449	1.986	0.180
8.283	4.980	0.698	0.170	0.702	0.066
5.987	3.856				
3.562	2.294				
1.959	1.190				
1.293	0.746				
0.499	0.320				
0.168	0.117				

Table S2. CO₂, CH₄ and N₂ adsorption-desorption equilibrium data at 303 K for [C₆MIM][B(CN)4]@ZIF-8 (low).

CO ₂ – 303 K		CH ₄ – 303 K		N ₂ – 303 K	
P (bar)	q _{exc} (mol/kg)	P (bar)	q _{exc} (mol/kg)	P (bar)	q _{exc} (mol/kg)
2.974	1.429	0.500	0.098	0.502	0.038
6.067	3.080	0.998	0.189	1.001	0.075
7.944	3.782	3.073	0.577	2.943	0.214
12.810	5.088	5.877	1.058	6.049	0.420
15.961	5.580	8.007	1.38	7.989	0.547
14.061	5.311	11.950	1.883	12.079	0.784
10.044	4.479	15.980	2.291	16.010	0.968
4.570	2.337	14.020	2.103	14.009	0.875
1.962	0.946	10.017	1.650	9.893	0.665
0.720	0.359	4.539	0.833	4.512	0.337
		1.939	0.369	1.986	0.158
		0.698	0.134	0.702	0.056

Table S3. CO₂ adsorption-desorption equilibrium data at 303 K for [C_nMIM][B(CN)₄]@ZIF-8 materials.

CO ₂ – 303 K						
[C ₆ MIM][B(CN) ₄]@ZIF-8 (low) - 2		[C ₂ MIM][B(CN) ₄]@ZIF-8 (low)		[C ₆ MIM][B(CN) ₄]@ZIF-8 (high)		
P (bar)	<i>q</i> _{exc} (mol/kg)	P (bar)	<i>q</i> _{exc} (mol/kg)	P (bar)	<i>q</i> _{exc} (mol/kg)	
0.151	0.064	0.499	0.212	0.151	0.055	
0.300	0.134	1.000	0.435	0.300	0.116	
0.517	0.240	3.035	1.342	0.517	0.203	
0.706	0.333	6.026	2.571	0.706	0.282	
0.850	0.405	7.995	3.207	0.850	0.342	
1.001	0.481	12.062	4.090	1.001	0.406	
2.096	1.051	15.881	4.589	2.096	0.878	
4.007	2.088	9.969	3.707	4.007	1.727	
6.972	3.502	4.519	2.010	6.972	2.918	
9.981	4.512	1.971	0.886	9.981	3.726	
5.334	2.772	0.699	0.337	5.334	2.294	
2.991	1.547			2.991	1.289	
1.502	0.745			1.502	0.628	
0.589	0.283			0.589	0.239	
0.098	0.046			0.098	0.042	

S2. Single-component CO₂,CH₄ and N₂ adsorption-desorption data of ZIF-8 and [C₆MIM][B(CN)₄]@ZIF-8 (low) at 273 K

Table S4. CO₂ adsorption-desorption equilibrium data at 273 K for pristine ZIF-8 and [C₆MIM][B(CN)₄]@ZIF-8 (low).

CO ₂ – 273 K			
ZIF-8		[C ₆ MIM][B(CN) ₄]@ZIF-8 (low)	
P (bar)	<i>q</i> _{exc} (mol/kg)	P (bar)	<i>q</i> _{exc} (mol/kg)
0.143	0.167	0.143	0.125
0.291	0.357	0.291	0.278
0.431	0.534	0.431	0.422
0.574	0.725	0.574	0.559
0.711	0.917	0.711	0.712
0.860	1.137	0.860	0.882
1.002	1.353	1.002	1.048
2.981	4.534	2.981	3.479
6.089	7.280	6.089	5.765
8.112	8.071	8.112	6.468
12.040	8.884	12.040	7.226
16.092	9.289	16.092	7.660
9.973	8.575	9.973	6.956
4.545	6.419	4.545	5.081
2.066	3.081	2.066	2.397
0.928	1.311	0.928	1.038
0.778	1.091	0.778	0.865
0.641	0.893	0.641	0.706
0.506	0.682	0.506	0.541
0.359	0.489	0.359	0.390
0.210	0.296	0.210	0.231
0.069	0.112	0.069	0.084