The details of the BG method:

The dimensions of simulation boxes:

- Series 1,2 and 3: 6.5 × 6.5 × 6.5 nm
- Series 1 x 1.125: 7.0 × 7.0 × 7.0 nm
- Series 1 x 1.25: 7.5 × 7.5 × 7.5 nm
- Series 1x 1.50: 8.5 × 8.5 × 8.5 nm

Periodic boundary conditions applied in all three dimensions.

Density of nodes: 200 × 200 × 200

Atom radius:

r_C =0.17 nm
r_O = 0.15 nm

Average effective micropore diameters from BG method were calculated using:

$$d_{mi,av} = \frac{\sum_{d \le 2\ \mathrm{nm}} d \cdot P(d)}{\sum_{d \le 2\ \mathrm{nm}} P(d)}$$

Table ESI 1. The average micropore diameters of all VPCs.

$d_{mi,av}$ [nm]											
S1_000	0.712	**S2_000**	0.712	**S3_000**	0.712	**S1_000x1.125**	0.875	**S1_000x1.25**	1.058	**S1_000x1.5**	1.461
S1_060	0.707	**S2_060**	0.707	**S3_060**	0.706	**S1_060x1.125**	0.864	**S1_060x1.25**	1.047	**S1_060x1.5**	1.445
S1_120	0.692	**S2_120**	0.703	**S3_120**	0.697	**S1_120x1.125**	0.848	**S1_120x1.25**	1.029	**S1_120x1.5**	1.417
S1_180	0.690	**S2_180**	0.692	**S3_180**	0.691	**S1_180x1.125**	0.841	**S1_180x1.25**	1.019	**S1_180x1.5**	1.405
S1_240	0.685	**S2_240**	0.681	**S3_240**	0.685	**S1_240x1.125**	0.830	**S1_240x1.25**	1.005	**S1_240x1.5**	1.390

Table ESI 2. Characteristics of simulation boxes. N_{H2O} is the number of water molecules in the simulation box having starting diameters $L_{box,x}$, $L_{box,y}$, and $L_{box,z}$, respectively. Method 1 – uses Gromax Genbox procedure, method 2 – simulation in water sphere.

Structure	*method 1*				*method 2*			
	N_{H20}	$L_{box,x}$	$L_{box,y}$	$L_{box,z}$	N_{H20}	$L_{box,x}$	$L_{box,y}$	$L_{box,z}$
		[nm]				[nm]		
carbonyl groups introduced randomly								
S1_000	3567	5.395	5.057	5.057	6252	6.500	6.500	6.500
S1_060	3701	5.418	5.114	5.133	6252	6.500	6.500	6.500
S1_120	3672	5.418	5.114	5.133	6252	6.500	6.500	6.500
S1_180	3659	5.429	5.115	5.133	6252	6.500	6.500	6.500
S1_240	3715	5.429	5.170	5.144	6252	6.500	6.500	6.500
carbonyl groups introduced randomly								
S2_000	3567	5.395	5.057	5.057	6252	6.500	6.500	6.500
S2_060	3551	5.406	5.057	5.057	6252	6.500	6.500	6.500
S2_120	3551	5.406	5.058	5.057	6252	6.500	6.500	6.500
S2_180	3534	5.406	5.058	5.068	6252	6.500	6.500	6.500
S2_240	3548	5.406	5.071	5.127	6252	6.500	6.500	6.500
carbonyl groups on the edges of structures								
S3_000	3567	5.395	5.057	5.057	6252	6.500	6.500	6.500
S3_060	3593	5.42	5.071	5.057	6252	6.500	6.500	6.500
S3_120	3713	5.42	5.18	5.078	6252	6.500	6.500	6.500
S3_180	3684	5.42	5.18	5.078	6252	6.500	6.500	6.500
S3_240	3671	5.42	5.18	5.109	6252	6.500	6.500	6.500
carbonyl groups introduced randomly – structures with shifted fragments								
S1_000x1.125	4847	5.886	5.433	5.494	n.a.			
S1_060x1.125	5111	5.909	5.528	5.570				
S1_120x1.125	5082	5.909	5.528	5.570				
S1_180x1.125	5055	5.920	5.529	5.570				
S1_240x1.125	5100	5.920	5.546	5.582				
carbonyl groups introduced randomly – structures with shifted fragments								
S1_000x1.25	6200	6.377	5.824	5.932	n.a.			
S1_060x1.25	6549	6.399	5.944	6.008				
S1_120x1.25	6526	6.399	5.944	6.008				
S1_180x1.25	6515	6.410	5.945	6.008				
S1_240x1.25	6530	6.410	5.958	6.019				
carbonyl groups introduced randomly – structures with shifted fragments								
S1_000x1.5	9918	7.359	6.653	6.806	n.a.			
S1_060x1.5	10367	7.381	6.773	6.882				
S1_120x1.5	10349	7.381	6.773	6.882				
S1_180x1.5	10335	7.392	6.787	6.893				
S1_240x1.5	10369	7.392	6.787	6.893				

Table ESI 3. The dependence between enthalpy of immersion and the percentage contents of oxygen. $-\Delta H_i = A_1 \cdot \{O\} + A_0$

Series	***method 1***		***method 2***	
	A_1 [J/g/%]	A_0 [J/g]	A_1 [J/g/%]	A_0 [J/g]
1	14.70	- 45.71	14.30	- 29.59
2	14.74	- 39.44	14.61	- 29.69
3	14.46	- 42.13	14.35	- 27.26
1 x 1.125	13.67	-14.78	-	-
1 x 1.25	13.57	19.09	-	-
1 x 1.50	13.45	31.89	-	-

Table ESI 4. The dependence between enthalpy of immersion and the polar surface area values.

$-\Delta H_i = B_1 \cdot S_{polar} + B_0$

Series	***method 1***		***method 2***	
	B_1 [J/m^2]	B_0 [J/g]	B_1 [J/m^2]	B_0 [J/g]
1	0.1699	- 50.38	0.1652	- 34.10
2	0.1714	- 41.76	0.1696	- 31.78
3	0.1592	- 43.05	0.1578	- 28.09
1 x 1.125	0.1245	- 18.20	-	-
1 x 1.25	0.1098	13.96	-	-
1 x 1.5	0.1072	30.13	-	-

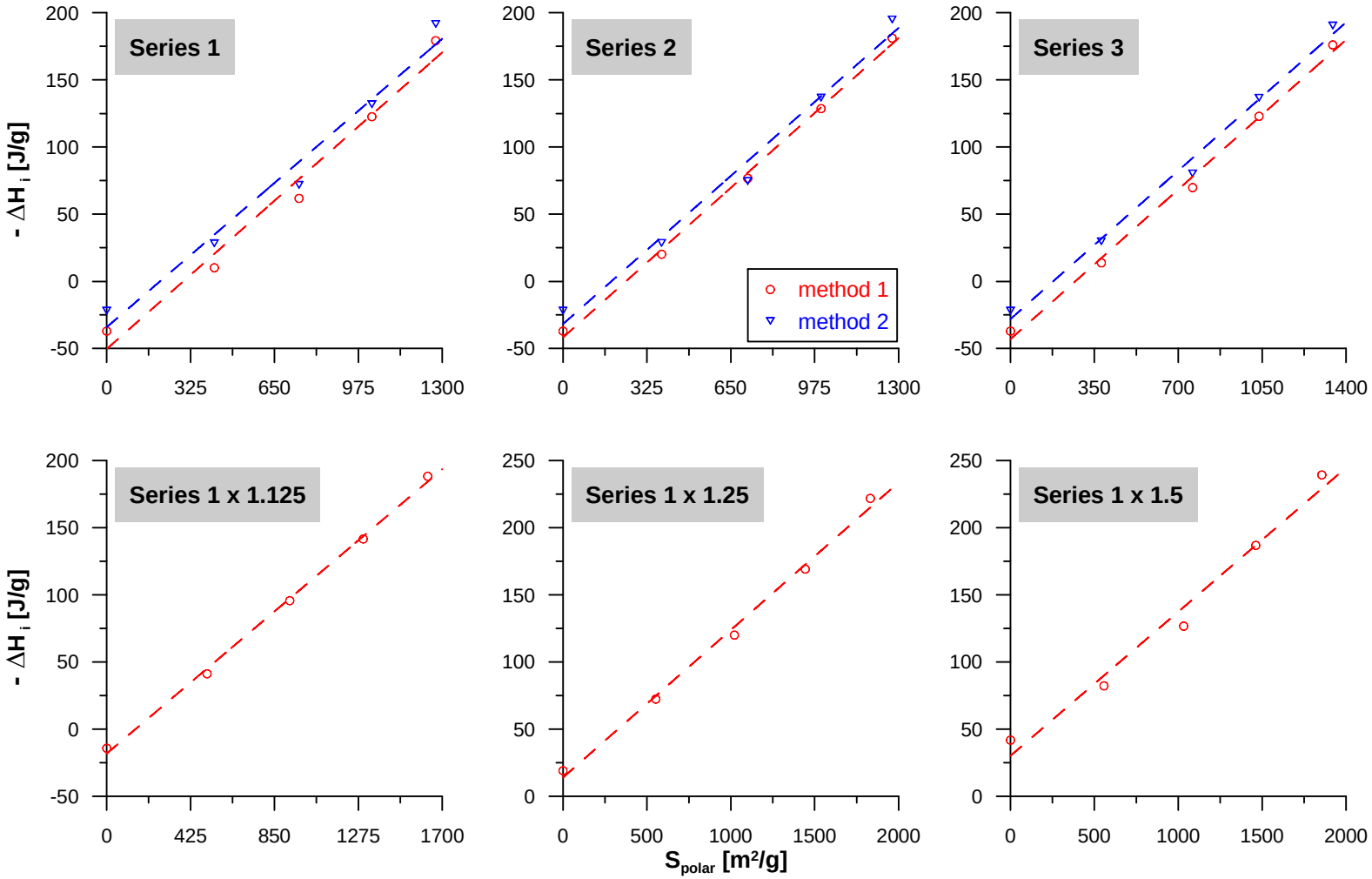

Figure ESI 1. The relation between enthalpy of immersion and polar surface area calculated from Vega ZZ.

Table ESI 5. The dependence between enthalpy of immersion and the ratio polar/nonpolar surface area.

$$-\Delta H_i = C_1 \cdot \frac{S_{polar}}{S_{nonpolar}} + C_0$$

Series	***method 1***		***method 2***	
	C_1 [J/g]	C_0 [J/g]	C_1 [J/g]	C_0 [J/g]
1	318.9	-32.89	310.9	-17.36
2	311.8	-22.22	312.9	-13.71
3	288.9	-24.27	287.3	-9.74
1 x 1.125	303.0	-1.13	-	-
1 x 1.25	305.7	28.98	-	-
1 x 1.5	309.4	43.62	-	-