Supporting information:

Hypothetical High-Surface-Area Carbons with Exceptional Hydrogen Storage Capacities: Open Carbon Frameworks

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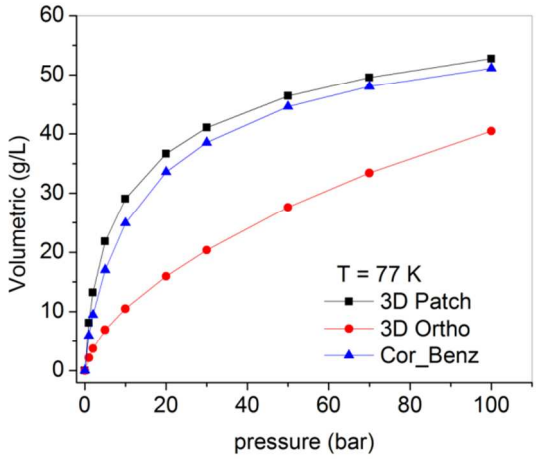
1. Parameters of the OCF adsorbents:

	3D Patch	**3D Ortho**	**Cor_Benz**
Density (g/cm^3)	0.48	0.16	0.38
Specific Surface (m^2/g)	3900 m^2/g	4400 m^2/g	6500 m^2/g
Energy of adsorption (average at T=77K)	3.9 kJ/mol	3.8 kJ/mol	3.2 kJ/mol
Energy of adsorption (maximal)	4.5 kJ/mol	4.5 kJ/mol	4.5 kJ/mol
Total capacity at 77 Kand 100 bar (g /kg)	115	260	131
Excess adsorption (maximum)at 77 K (g/kg)	74 (at ~45 bar)	85 (at ~65 bar)	83 (at ~50 bar)
Total capacity at 300 K and 100 bar (g /kg)	18	47	17.5

Comments:

a) The difference between specific surfaces of 3D Patch and 3D Ortho structures is a consequence of different orientations of bonded supra-molecules, which results in different accessible surface of the supra-molecule edges.

b) The average energy of adsorption is a consequence of the energy distribution due to the edge contribution

c) High total capacity of 3D Ortho structure is a consequence of low density and important gas contribution in the pore volume

2. Volumetric capacity in OCF: