Adsorption of carbon dioxide, methane, and their mixtures in porous carbons: effect of surface chemistry, water content, and pore disorder

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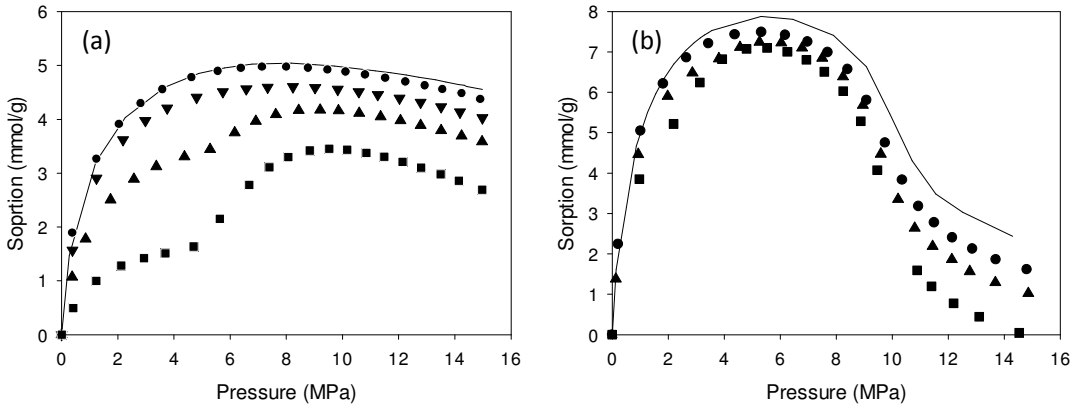

Figure S1 (a) Experimental excess adsorption isotherms for carbon dioxide at 318.15 K on the Filtrasorb F400 activated carbon with different amounts of preadsorbed water: (circles) 0.49 mmol(H_2O)/g, (triangles) 2.22 mmol(H_2O)/g, (squares) 5.26 mmol(H_2O)/g, (stars) 12.6 mmol(H_2O)/g. (b) Experimental excess adsorption isotherms for methane 318.15 K on the Filtrasorb F400 activated carbon with different amounts of preadsorbed water: (circles) 0.46 mmol(H_2O)/g, (triangles) 1.11 mmol(H_2O)/g, (squares) 5.22 mmol(H_2O)/g, (stars) 12.8 mmol(H_2O)/g. The black solid line shows the methane adsorption isotherm in dry condition.

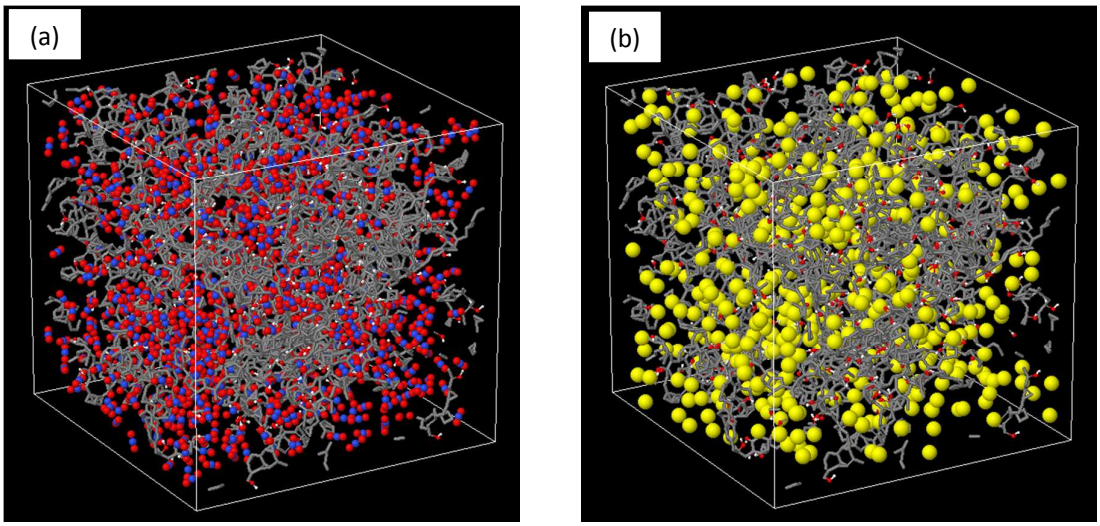

Figure S2. (a) Typical molecular configuration for carbon dioxide adsorbed at T= 318.15 K and p = 15 MPa on CS1000AF. (b) Typical molecular configuration for methane adsorbed at T= 318.15 K and p = 15 MPa on CS1000AF. The sticks are C-C, C-H and C-O bonds. Red and white spheres are the oxygen and hydrogen atoms, respectively. Blue spheres and yellow spheres are the carbon atoms of the carbon dioxide molecules and the methane molecules, respectively.

Table S1. Lennard-Jones interaction parameters, partial charges and bond parameters for water, carbon dioxide, methane and nitrogen.

Molecule	ε (K)	σ (nm)	q (e)	l (nm)	θ (°)
Water					
O – O	78.21	0.3167	-0.82		
H – H	---	---	+0.41		
O – H	---	---		0.1	
H – O – H					109.47
Carbon dioxide					
C – C	28.129	0.2757	+0.6512		
O – O	80.507	0.3033	-0.3256		
C – O	47.588	0.2892		0.1149	
O – C – O					180.0
Methane					
CH_4	148.1	0.381			
Nitrogen					
N_2	95.2	0.375			

Table S2. Lennard-Jones interaction parameters and partial charges for CS1000A and CS1000AF atoms and groups.

Atom or group	ε (K)	σ (nm)	q (e)
Carbon without heteroatom			
C	28	0.34	-
Hydroxyl			
C	33.214	0.35	+0.265
O	85.550	0.312	-0.683
H	--	--	+0.418
C-H group			
C	33.214	0.35	-0.06
H	15.097	0.25	0.06

Table S3. Bond parameters for CS1000AF model

Group	l (nm)	θ (°)
Hydroxyl		
C-O	0.1364	--
O-H	0.096	--
C-O-H	--	113
C-H group		
C-H	0.109	--