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Supporting Information

Carbon Dioxide Capture Enhanced by Pre-Adsorption of Water and Methanol in UiO-66

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Models of the molecules:

a) Carbon dioxide

Nonbonded interactions			
(pseudo)atom	ε/k_B [K]	σ [Å]	q [e]
C	29.933	2.745	0.6512
O	85.671	3.017	-0.3256
Bond lengths			
$r_{O=C}$ [Å]		$r_{C=O}$ [Å]	
1.15		1.15	
Bond Angles			
$\alpha_{O=C=O}$ [deg]			
180			

b) Nitrogen

Nonbonded interactions			
(pseudo)atom	ε/k_B [K]	σ [Å]	q [e]
N	38.298	3.306	-0.40484
M	-	-	0.8096
Bond lengths			
$r_{N\equiv N}$ [Å]		r_{N-M} [Å]	
1.1		0.55	
Bond Angles			
α_{N-M-N} [deg]			
180			

c) Methanol

Nonbonded interactions			
(pseudo)atom	ε/k_B [K]	σ [Å]	q [e]
CH_3	98	3.75	0.265
O	93	3.02	-0.7
H	0	0	0.435
Bond lengths			
r_{CH3-OH} [Å]		r_{O-H} [Å]	
1.43		0.945	
Bond Angles			
$\alpha_{CH3-O-H}$ [deg]		k_α/k_B [K/rad]	
108.5		55400	

d) Water

Nonbonded interactions			
(pseudo)atom	ε/k_B [K]	σ [Å]	q [e]
O	81.899	3.16	0
M	-	-	-1.048
H	-	-	0.524
Bond lengths			
r_{O-M} [Å]		r_{O-H} [Å]	
0.125		0.957	
Bond Angles			
α_{H-O-H} [deg]		α_{H-O-M} [deg]	
104.52		52.26	

Results:

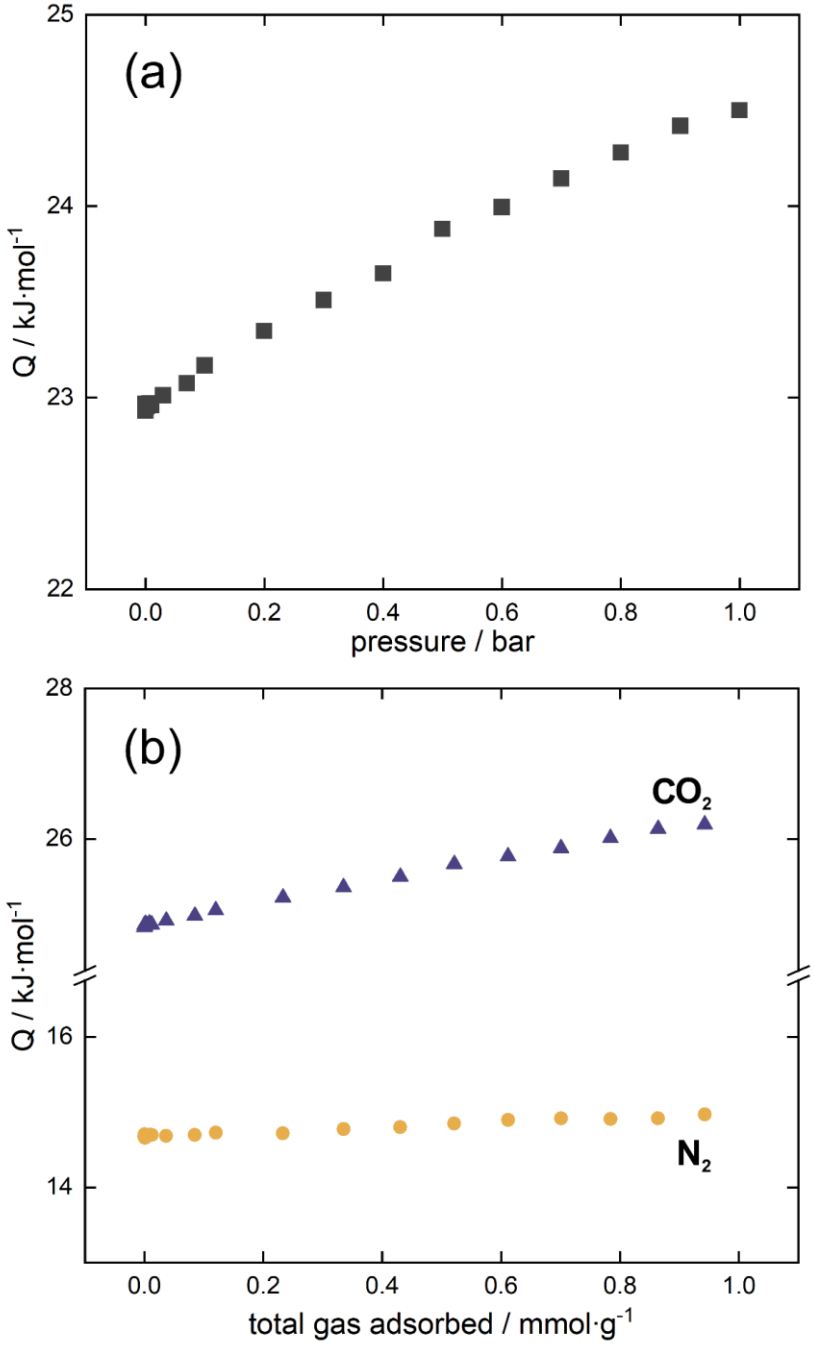

Figure S1. Heat of adsorption of the mixture of CO_2 and N_2 (a) and individual components (b) in UiO-66.

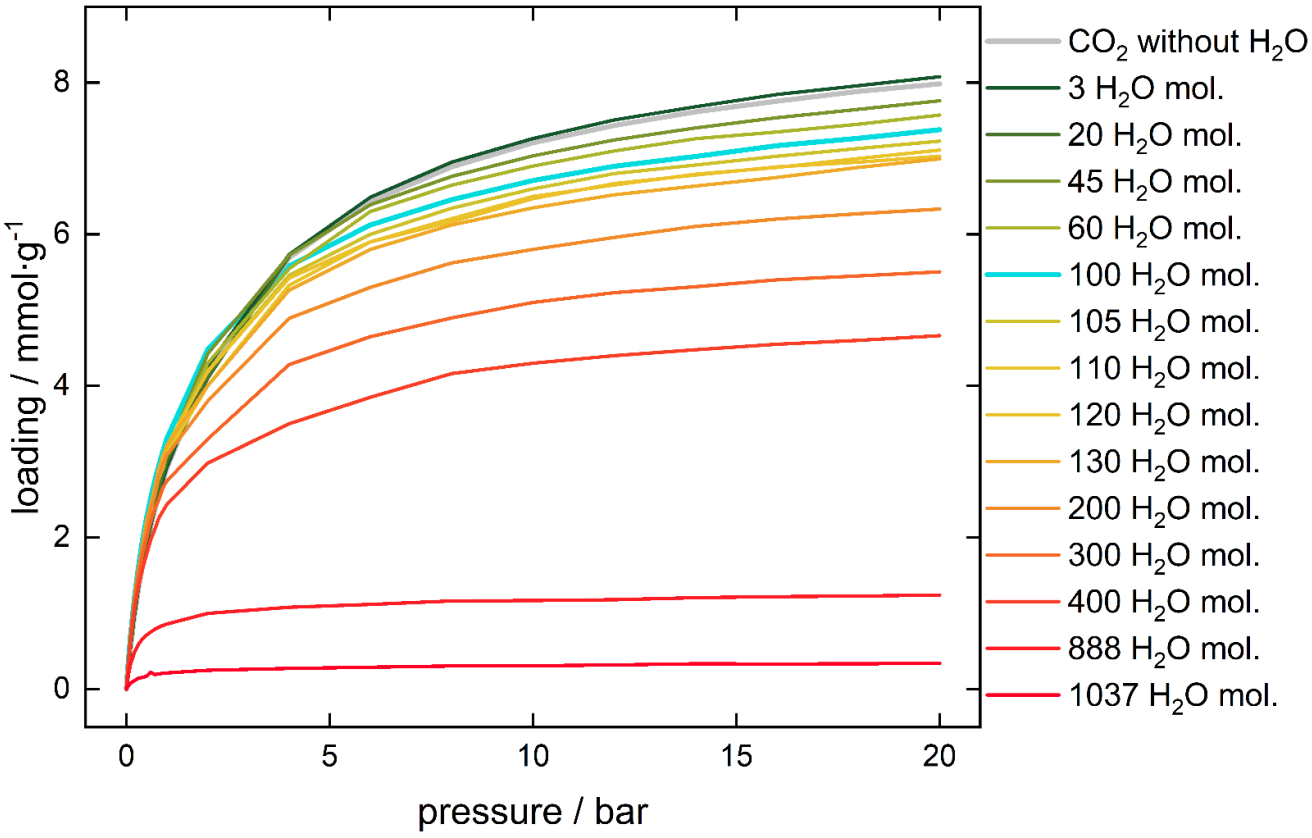

Figure S2. Adsorption isotherms of carbon dioxide with different content of water in pores of UiO-66 from 0 to 20 bar. Grey line stand for CO_2 adsorption, cyan line stand for an isotherm with pre-adsorbed 100 molecules of water per unit cell.

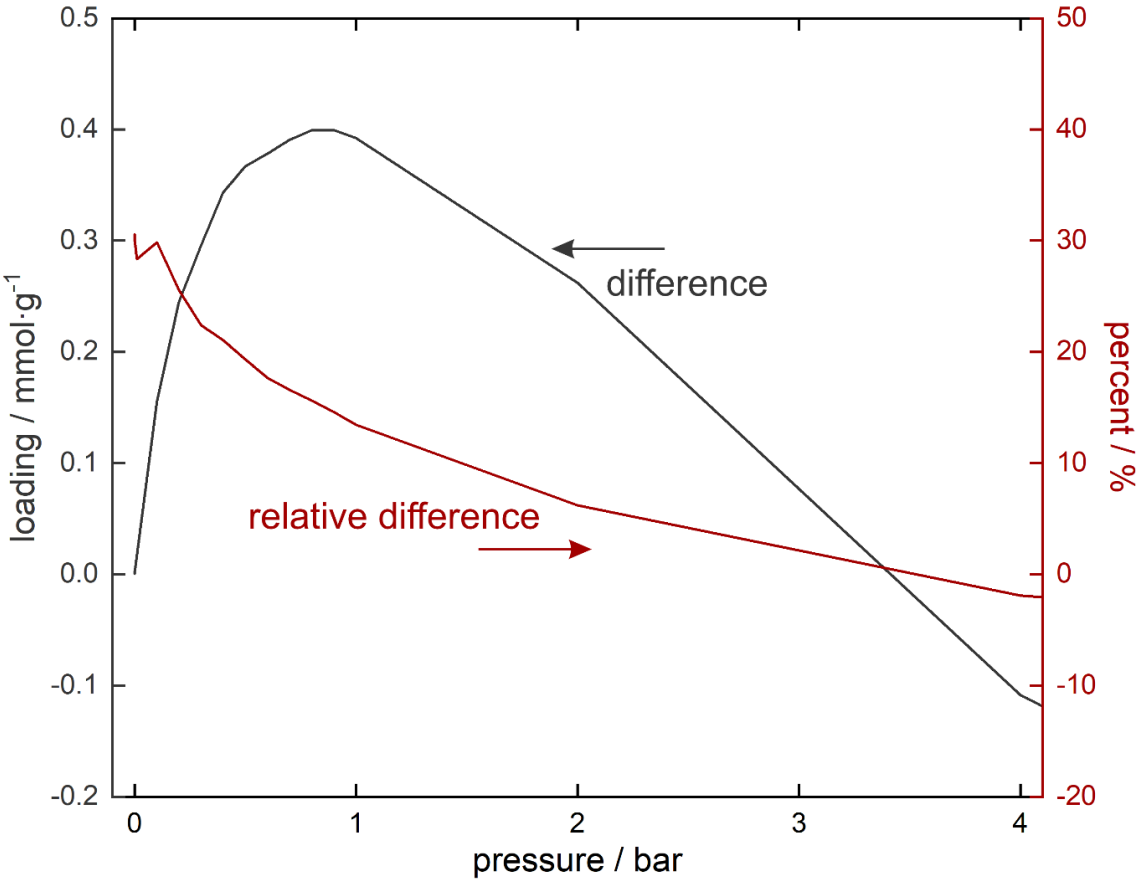

Figure S3. Difference (grey) and relative difference (red) between carbon dioxide adsorption and carbon dioxide with pre-adsorbed 1.8 mmol·g^{-1} of water.

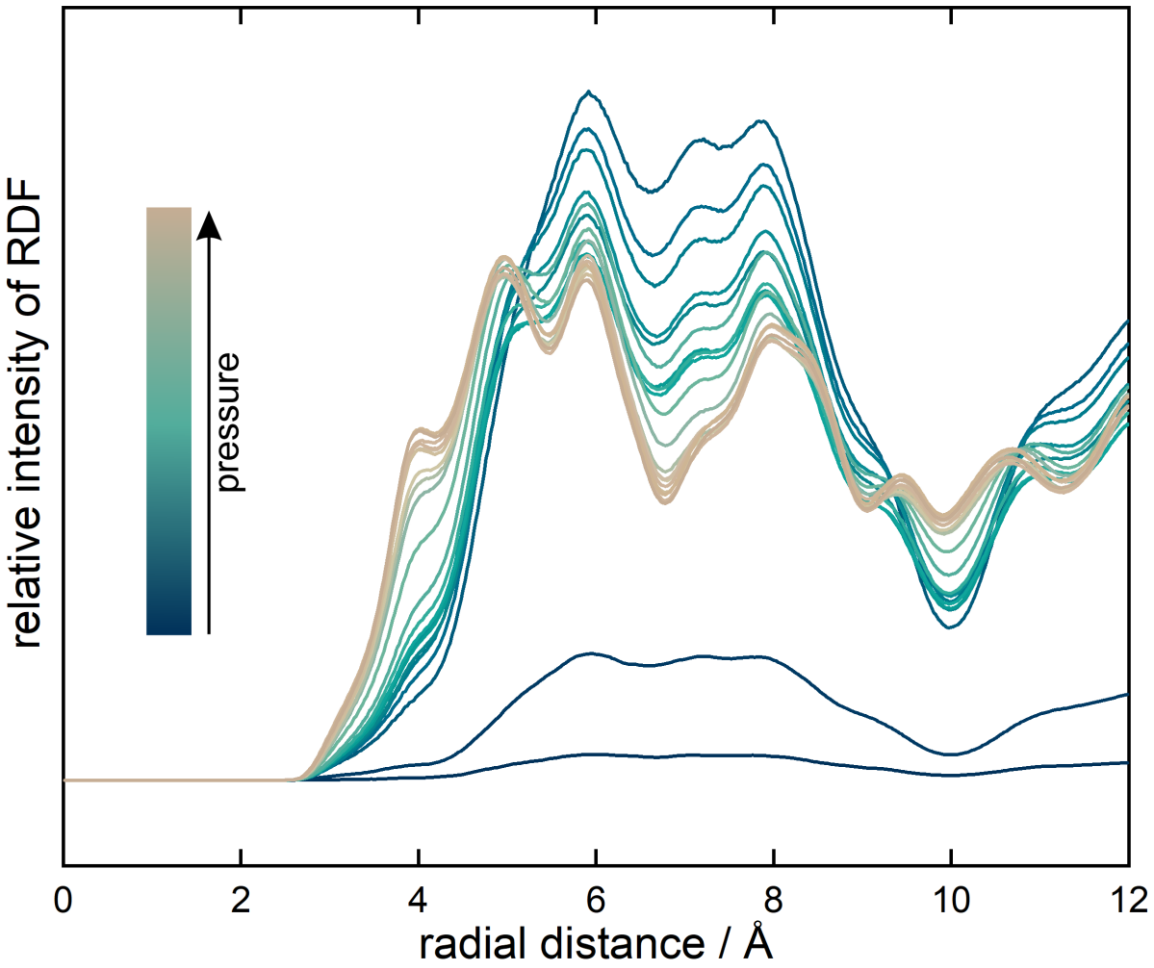

Figure S4. Radial distribution functions between the oxygen atom from water and the carbon atom from carbon dioxide in rising pressure from 0 to 20 bar.

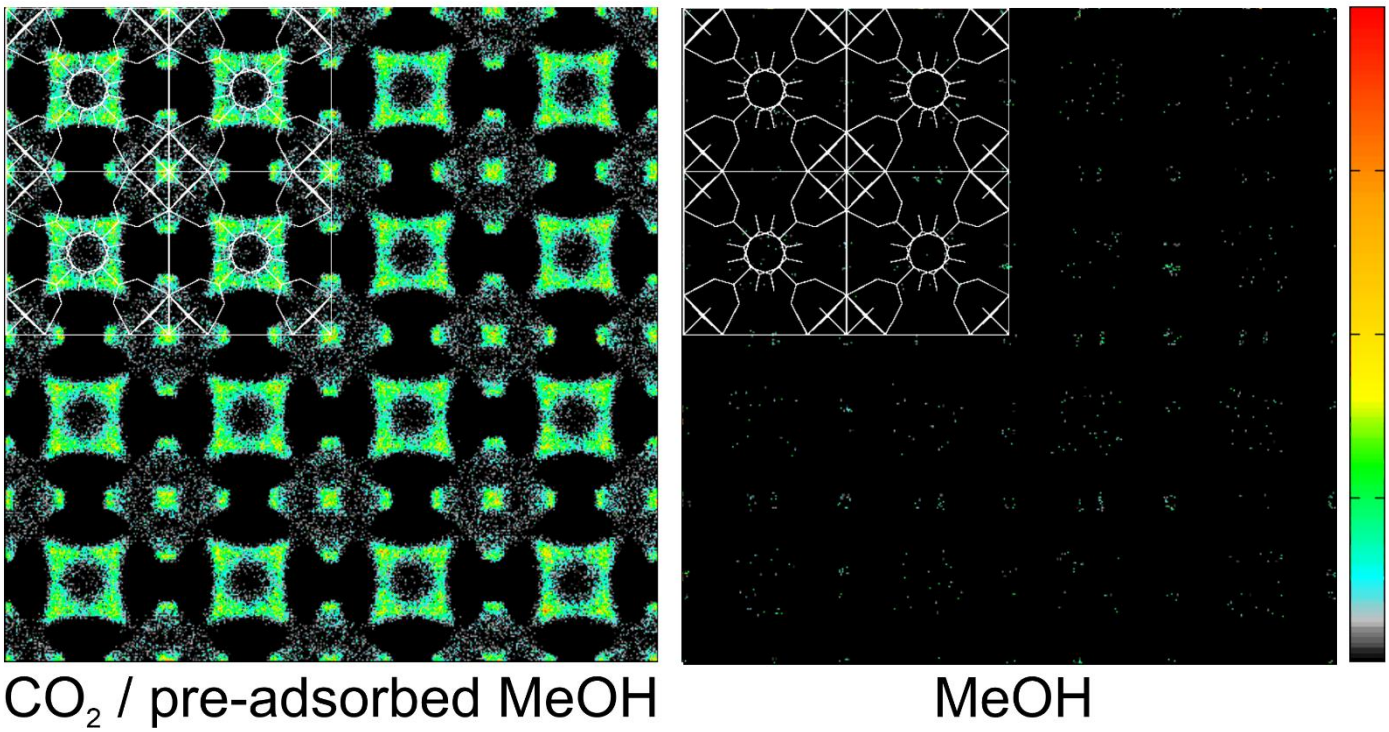

Figure S5. Average occupational density profiles of: 0.1 mmol·g^{-1} of methanol (right) and carbon dioxide with pre-adsorbed 0.1 mmol·g^{-1} of methanol (left) at 20 bar. For better observation of the effect, methanol molecules were not included in the left figure. The schemes of the structure and color scale are also included.