Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Enhanced mechanical strength of zeolites by adsorption of guest molecules

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Table S1. Forcefield parameters used to describe the CO_2 – CO_2 and CO_2 - silicalite SiO_2 interactions. The cross-parameters for the Lennard-Jones potential are obtained using the Lorentz-Berthelot combining rules. The charges and Lennard-Jones parameters for are taken from the work by Harris and Yung and Carre et al.

Molecule	σ **(nm)**	ε/k_B **(K)**	q **(e)**	l **(nm)**	θ **(deg)**
carbon dioxide					
C – C	0.2757	28.129	+0.6512		
O – O	0.3033	80.507	-0.3256		
C – O	0.2892	47.588		0.1149	
O – C – O					180°
SiO_2					
Si – Si	3.7950	0.533600	+1.910418		
O – O	3.1540	0.648700	-0.955209		

Table S2. Forcefield parameters used to describe SiO_2 Buckingham interactions in silicalite. The parameters are taken from the work by Carre et al.

Molecule	***A*** **(eV)**	***B*** **(Å^{-1})**	***C*** **(eV.Å^6)**
Si – Si	3150.462646	2.851451	626.751953
Si – O	27029.419922	5.158606	148.099091
O – O	659.595398	2.590066	26.836679

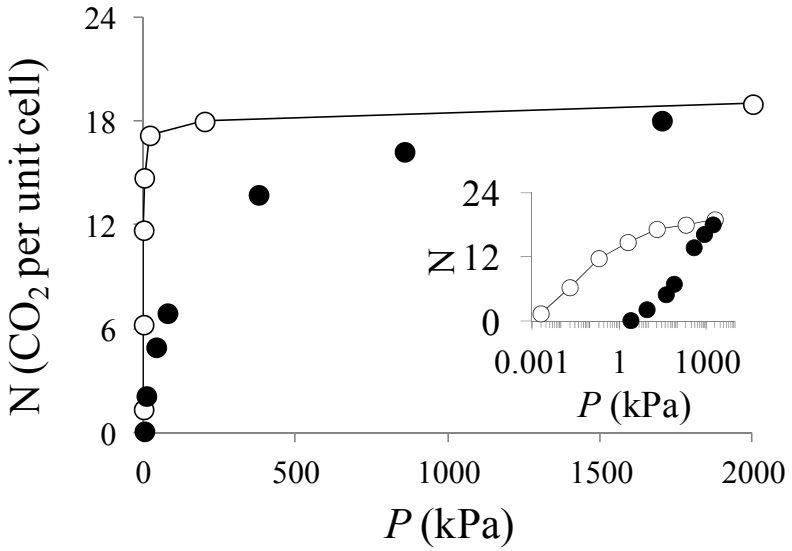

Figure S1. CO_2 adsorption isotherm at T = 303 K in silicalite: (black symbols) simulated data from this work, (open symbols) experimental data taken from Ref. 26. The insert shows the same data with pressures in a log scale.

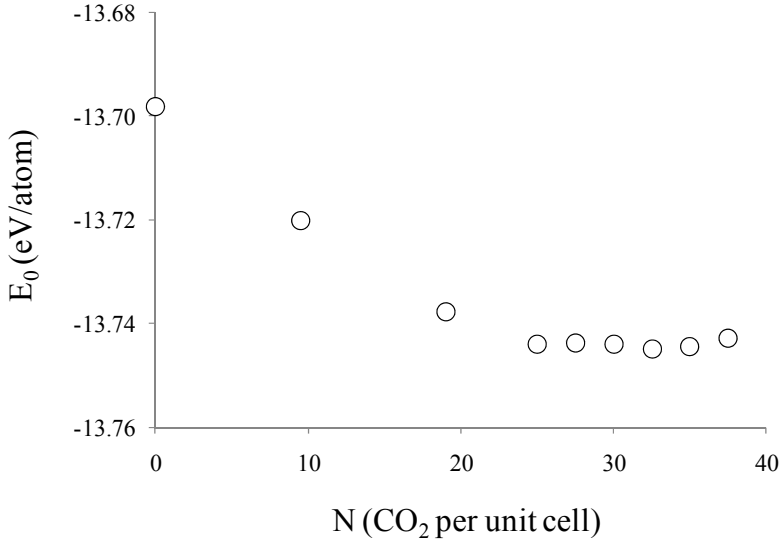

Figure S2. Energy E_0 per zeolite atom (Si or O) for silicalite loaded at room temperature with CO_2 as a function of the number of adsorbed molecules N_{CO2}.