Supplementary Material (ESI) for Chemical Communications

Structural changes in nanoporous solids due to fluid adsorption: thermodynamic analysis and Monte Carlo simulations.

Electronic supplementary information

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Dispersion-repulsion interactions :

All the dispersion-repulsion interactions were modelled with a Lennard-Jones potential:

$$U_{ij} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right]$$

The parameters are given in table S1.

	σ (A)	ε (K)
Cl-Cl	3.50	193.8
C-C	3.35	64.0
H-H	2.64	12.0
Cl-O_{host}	3.275	107.8
C-O_{host}	3.175	64.0
H-O_{host}	2.82	30.43

Table S1: Forcefield parameters for LJ potential

All the non given parameters can be obtain by using the Lorentz-Berthelot mixing rules (arithmetic rule for σ and geometric rule for ε). No dispersion terms were taken into account with silicon atoms (Kiselev approximation).

Charges parameters :

Electrostatic charges of the framework were set to -0.7e for the oxygen and 1.4e for the silicon atom.

Adsorbate charges parameters are given in figure S1.

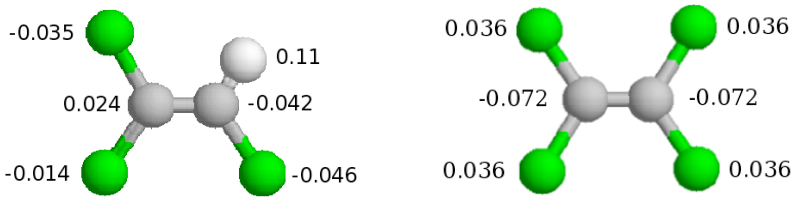

Fig S1 : Atomic charges (in electron units) used for Trichloroethene and Tetrachloroethene in Monte-Carlo simulations.