

## 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:

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

The parameters are given in table S1.

	$\sigma$ (Å)	$\epsilon$ (K)
Cl-Cl	3.50	193.8
C-C	3.35	64.0
H-H	2.64	12.0
Cl-O <sub>host</sub>	3.275	107.8
C-O <sub>host</sub>	3.175	64.0
H-O <sub>host</sub>	2.82	30.43

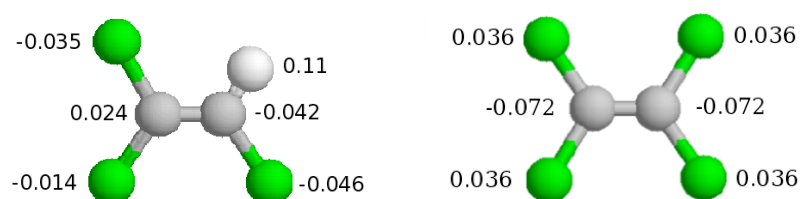
**Table S1:** Forcefield parameters for LJ potential

All the non given parameters can be obtain by using the Lorentz-Berthelot mixing rules (arithmetic rule for  $\sigma$  and geometric rule for  $\epsilon$ ). 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.