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:

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

The parameters are given in table S1.

<table>
<thead>
<tr>
<th></th>
<th>(\sigma) (Å)</th>
<th>(\varepsilon) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cl-Cl</td>
<td>3.50</td>
<td>193.8</td>
</tr>
<tr>
<td>C-C</td>
<td>3.35</td>
<td>64.0</td>
</tr>
<tr>
<td>H-H</td>
<td>2.64</td>
<td>12.0</td>
</tr>
<tr>
<td>Cl-O\textsubscript{host}</td>
<td>3.275</td>
<td>107.8</td>
</tr>
<tr>
<td>C-O\textsubscript{host}</td>
<td>3.175</td>
<td>64.0</td>
</tr>
<tr>
<td>H-O\textsubscript{host}</td>
<td>2.82</td>
<td>30.43</td>
</tr>
</tbody>
</table>

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 \(\varepsilon\)). 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.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Atomic charges (in electron units) used for Trichloroethene and Tetrachloroethene in Monte-Carlo simulations.}
\end{figure}