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1. Introduction & Methodology

Structural and dynamical properties of fluid ethane confined within silica nanopores have been investigated by Molecular Dynamics simulations. The pure ethane phase and equimolar mixtures of ethane and CO\textsubscript{2} were considered; at densities in the range \( \rho / \rho_{\text{crit}} = 0.05 - 2.18 \).

- Molecular Dynamics simulations, times \( \sim 60 \text{ ns} \).
- Microcanonical Ensemble NVE, at \( T \sim 320 \text{ K} \).

2. Structural Properties: Local Densities

**Densities along \( z \):**

\[
\begin{array}{c|c|c}
\rho_{\text{Ethane}} & \rho_{\text{CO}_2} \\
\hline
2.28 & 1.35 \\
2.00 & 0.70 \\
2.00 & 0.46 \\
1.50 & 0.25 \\
\end{array}
\]

**Densities along \( r \):**

**Excess sorption densities:**

\[
\Delta \rho_{\text{exc}} = \langle \rho_{\text{pore}} \rangle - \rho_b
\]

Density profiles reveal the formation of a dense adsorption layer, rich in CO\textsubscript{2}.

3. Structural Properties: Orientations

**Orientation wrt the silica wall:**

- Interfacial Ethane \( \rightarrow \) parallel to surface.
- Interfacial CO\textsubscript{2} \( \rightarrow \) bimodal distribution, parallel and perpendicular to surface. Due to directional hydrogen-bond like interactions \( \text{H-O-Si} \), with the silica walls.
- Bulk region \( \rightarrow \) no preferential orientations.

**Orientational function:**

\[
G_2(r) = \langle \rho_i \cdot \rho_j \rangle \delta(r - r_i) - 1
\]

\( G_2 < 0 \) at small \( r \) \( \rightarrow \) T-shaped configurations;

\( G_2 \approx 0.2 \) at \( r \sim 3 - 4 \text{ Å} \) \( \rightarrow \) intermediate between T-shaped and parallal arrangements.

4. Dynamical Properties

**Diffusion:** Self-diffusion coefficients were computed from the classical Einstein relation for the mean squared displacements.

<table>
<thead>
<tr>
<th>( \rho_b / \rho_c )</th>
<th>Ethane ( D_{\text{bulk}} )</th>
<th>CO\textsubscript{2} ( D_{\text{bulk}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>20.8</td>
<td>2.71</td>
</tr>
<tr>
<td>0.46</td>
<td>7.44</td>
<td>2.25</td>
</tr>
<tr>
<td>0.70</td>
<td>6.99</td>
<td>1.85</td>
</tr>
<tr>
<td>1.35</td>
<td>4.91</td>
<td>1.88</td>
</tr>
<tr>
<td>2.28</td>
<td>3.15</td>
<td>1.43</td>
</tr>
<tr>
<td>2.70</td>
<td>1.60</td>
<td>1.15</td>
</tr>
</tbody>
</table>

**Local diffusion along \( r \):**

\[
D_{\text{eff}} = \langle \rho_i \cdot \rho_j \rangle \delta(r - r_i) - 1
\]

**Diffusion is reduced under confinement and increasing Pressure.**

**Incorporation of CO\textsubscript{2} into the fluid enhances the diffusion of ethane species.**

**Coexistence of fast and slow translational modes within the cavity.**

**Orientational correlations of interfacial molecules decay more slowly than bulk-like ones; CO\textsubscript{2} correlations being the slowest.**

5. Conclusions

Preferential adsorption of CO\textsubscript{2} over ethane within the adsorbed layer inside the pores led to significant increments in ethane mobility, due to displacements of interfacial ethane molecules towards more internal, bulk-like, locations. These effects were found to be more pronounced at low densities and under strong confinement.