Computational investigation of the effect of \( n \)-alkane chain length on the alkane/water interfacial width

Collin D. Wick, Louisiana Tech University, Ruston, LA

<table>
<thead>
<tr>
<th>Alkane</th>
<th>Interfacial Width</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n )-hexane</td>
<td>3.15 Å</td>
</tr>
<tr>
<td>( n )-nonane</td>
<td>2.90 Å</td>
</tr>
</tbody>
</table>

Direct comparisons with x-ray reflectivity experiments were made. Computational results show that alkane interfacial width increases with longer alkanes, in contrast to experiment.