

**Computational Study of n-Alkane/Water Interface: The Role of Alkyl Chain Length on Interfacial Width and Ion Distributions compared with Air/Water Interface**

*Oneka T. Cummings and Collin D. Wick*

*Department of Chemistry, Louisiana Tech University, Ruston, Louisiana, 71270*

The interfacial behavior of aqueous species, such as ions, may be affected by the nature of the hydrophobic liquid with which water comes into contact. A molecular level understanding of how specific hydrophobic liquids influence the interfacial properties of water will benefit ion complexation, phase transfer catalysis, and many other applications. In this study, molecular dynamics simulations of *n*-alkane/water systems are carried out at 298K with polarizable interactions. We investigate the *n*-alkane-water interface, the effect of changing the length of the alkane chain and size of the alkane region on the water/alkane interfacial width. We also compared sodium-halide ion distributions at the *n*-octane-water and air-water interfaces. Alkane-water interfaces with linear alkanes of different chain lengths had fairly similar properties, except that with longer alkanes, the interfacial width decreased. The interfacial widths for both water and the alkanes decrease with increasing alkane chain length. X-ray reflectivity experiments have been known to observe the opposed trend, that increasing the alkane chain length increased the interfacial width. Since these experiments are related to electron densities and not specific densities which we used in our initial investigation, we extended our study to calculate interfacial width based on electron densities and mimic the capillary wave action which is included at the macroscopic level. We modeled *n*-hexane-water and *n*-nonane-water and came to the same conclusions here as well; the longer alkane chain had a shorter interfacial width. Also, varied system sizes of the alkane region seemed to have no significant effect on the alkane-water interfacial width. Sodium-halide concentrated solutions at the *n*-octane-water interface were simulated and compared with the air-water interface. Bromide and chloride showed significantly reduced interfacial concentration at the alkane-water interface. Iodide, in contrast, had similar interfacial concentrations at both interfaces which is attributed to the fact that it has favorable hydrophobic interactions with alkanes that were not as strong for bromide and chloride with the alkanes.