Self-accumulation of aromatics at oil-water interface: A molecular dynamics study

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The interface between two immiscible liquids is a noncentrosymmetric environment about which we know very little in comparison with other condensed-matter materials and their surfaces. Experimental probes of liquid-liquid interfaces are limited because of the relatively small size---typically only a few molecular diameters wide and the buried nature of the interface. Here we have investigated the water and a light-oil model interface. It was found that aromatics concentrate on the interfacial regions, whereas the other hydrocarbons of oil are uniformly distributed along the oil slab. We attributed the self-accumulation of the aromatics to the favorable Gibbs free energy due to the lower interfacial tension between the aromatics-water interfaces. Further, we suggest that the 'weak hydrogen bonding' between the aromatic rings and the proton of the water are the cause of the lower interfacial tension among others.

First principles simulations of liquid-vapor interfaces: Structures, dynamics and chemical reactivity

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Aqueous interfaces are ubiquitous and fundamentally important in understanding many atmospheric, biological, and geological systems. In realistic environments, presence of impurities or surfactants can subtlely change many interfacial properties. Naturally, many experimental and theoretically studies has utilized small amphiphilic molecules like methanol to serve as a model surfactant while probing the liquid-vapor interface in order to understand how surfactants can alter different interfacial properties. Here, we will utilize first principles simulations using density functional theory with various exchange and correlation functionals as well as van der Waals corrections. The accuracy of first principles simulations utilizing different sampling techniques (MD and MC) in predicting bulk properties of a range of fluids will first be discussed. Second, structural and dynamical changes at the interface as a function of increase methanol coverage will be presented. Last, how interfacial water can affect and and alter reaction kinetics in the vicinity of the interface will be shown.

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