

~~Special Polymer Physics Seminar ~~

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301 Steidle Bldg.

Air-Liquid Interface of Imidazolium-Based [Tf₂N⁻] Ionic Liquids: Insight from Molecular Dynamics Simulations

Room-temperature ionic liquids (RTILs) are salts in the liquid state at ambient temperatures. They typically consist of bulky and asymmetric organic cations and inorganic or organic anions. In contrast to simple molten salts, the molecular asymmetry built into the ions (usually cations) opposes the strong charge ordering due to the ionic interactions that normally causes crystallization in the simple molten salts, and therefore, RTILs exhibit a wide liquid range. An enormous number of different RTILs can be prepared and their thermophysical properties can be fine-tuned by variations in the molecular structures of the cations and anions, as well as by mixing and matching different ion pairs. RTILs have a variety of unique properties including a very small (though non-zero) vapor pressure, good thermal stability, favorable solvation behavior, and high reactivity and selectivity.

Recently, RTIL membranes have been suggested for separation of volatile organic compounds (VOC) from air. Such the separation process is environmentally friendly since a contamination of the environment by RTILs is improbable due to their high chemical stability and negligible vapor pressure. Relatively high molecular diffusion occurring in RTILs allows high mass fluxes through a membrane and variability of chemical properties of RTILs enables to synthesize a convenient RTIL for a particular separation process. The RTILs also exhibit a long life and a possibility to recycle used RTILs. In the RTIL membranes, VOC molecules pass through the air-liquid interface and the understanding of the nature and structure of the interface is therefore important for rational membrane design. Properties such as orientation of the cations and anions, density behavior with respect to the interface normal, and relative population of the cations and anions at the interface all affect the dynamics of adsorption of VOC molecules and their absorption into the bulk phase.

In my talk, I will present molecular dynamics simulations of the air-liquid interface of three room temperature ionic liquids with a common anion: bis(trifluoromethylsulfonyl) imide, and imidazolium-based cations that differ in the alkyl tail length: 1-butyl-3-methylimidazolium, 1-hexyl-3-methylimidazolium, and 1-octyl-3-methylimidazolium. The surface tension was computed using the mechanical route and its value slightly overpredicts experimental values. The air-liquid interface was analyzed using the intrinsic method of Identification of the Truly Interfacial Molecules. The structural and dynamic properties of the interfacial, sub-interfacial and bulk layer were determined and will be discussed.