Structure and Hydrogen Bonds of Hydrophobic Deep Eutectic Solvent-Aqueous Liquid-Liquid Interfaces

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Abstract

Hydrophobic deep eutectic solvents (DESs) emerge as candidates to extract organic substrates from aqueous solutions. The DES-aqueous liquid-liquid interface plays a vital role in the extraction ability of hydrophobic DES because the non-bulk structure of molecules at the interface could cause thermodynamic and kinetic barriers. One question is how the DES compositions affect the structural features of the DES-aqueous liquid-liquid interface. We investigate the density profile, dipole moment and hydrogen bonds of eight hydrophobic DES-aqueous liquid-liquid interfaces using molecular dynamics simulations. The eight DESs are composed of four organic compounds: decanoic acid, menthol, thymol, and lidocaine. The simulation results show the variations of dipole moment and hydrogen bond structure and dynamics at the liquid-liquid interfaces. Such variations could influence the extraction ability of DES through adjusting the partition and kinetics of organic substrates in the DES-aqueous biphasic systems.

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