Phase separation in hydrocarbon-alcohol-water systems at the molecular level: A first-principles-based theoretical study

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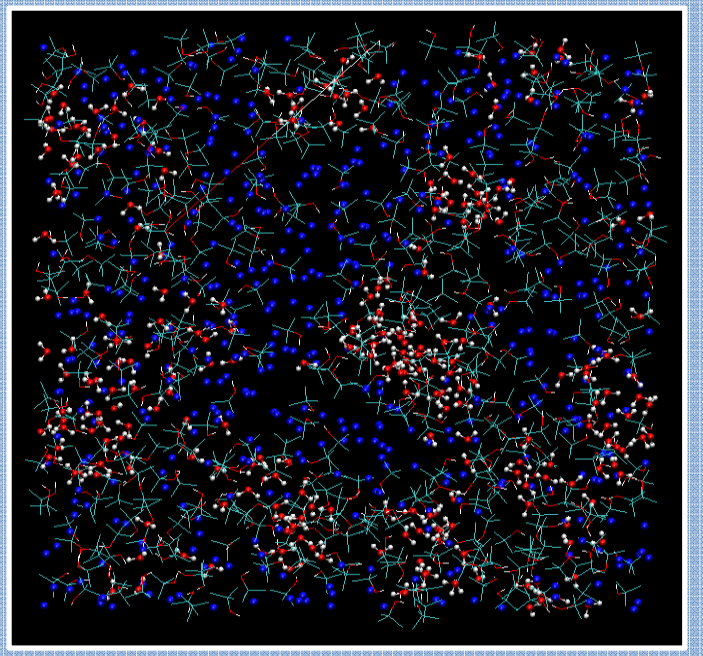
A key constraint for achieving the extensive use of alcohols as an addition to automotive fuels is liquid-liquid phase separation in hydrocarbon-alcohol mixtures that is exacerbated by the presence of water, as shown on the right in methane-methanol-water mixture. Understanding the mechanisms of liquid-liquid phase separation is impossible without a detailed molecular-level picture of the morphology and dynamics of alcohol-hydrocarbon-water systems. The objective of this proposal is to deduce patterns of the self-aggregation of alcohols in hydrophobic and hydrophilic media and to identify the microscopic origins of phase separation in alcohol-hydrocarbon mixtures, by using the first-principle-based effective fragment potential (EFP) method.

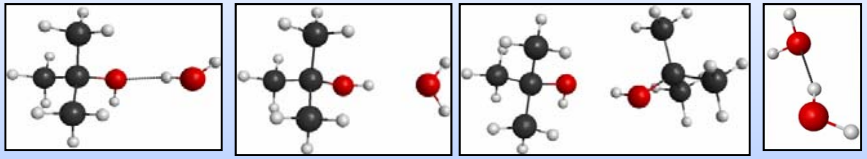


On the example of water-tert-butanol mixtures we showed that the structure of complex liquid is very sensitive to a quality and balance in description of intermolecular interactions; structures and radial distribution functions obtained by EFP are in agreement with neutron diffraction data.

Our next goals will include investigation of hydrophobic water interfaces and influence of ions on water-alcohol interactions.

Water-TBA mixtures: from clusters to bulk

Comparison of EFP and MP2 interaction energies (kcal/mol) and EFP-MD simulations of equal molar water-TBA liquid



	O-HW	H-OW	O-H	OW-HW
EFP	-7.4	-5.4	-7.9	-5.9
MP2	-7.3	-6.3	-8.3	-6.0