Aggregation in Surfactant-Free Ternary Mixtures

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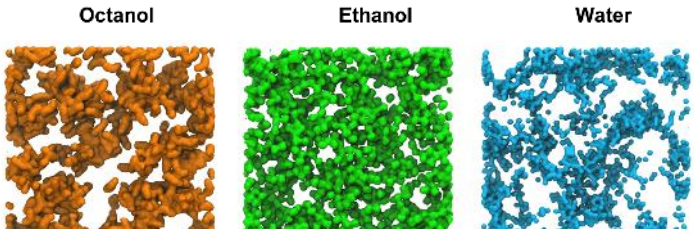
In recent years it has become more and more evident that presumably simple solutions can show a variety of nanoscale aggregation structures. Ternary mixtures of three liquids, in which two show only partial mutual solubility, resemble different types of microemulsions even in the absence of classical surfactants. We present fully atomistic molecular dynamics simulations of octanol/ethanol/water mixtures, a typical representative of these "surfactant-free microemulsions". We compare MD simulations results with experimental SAXS/WAXS and neutron scattering data and present a detailed analysis of the observed structures. We recognize three types of microemulsions: i) a direct oil-in-water microemulsion consisting of octanol rich aggregates in a water rich phase, ii) a bicontiuous sponge-like microemulsion, and iii) a reverse water-in-oil mircoemulsion, in which the polar phase comprises a network of hydrogen bondend structures.



1A 2 nm thick slice through a snapshot of an octanol/ethanl/water mixture in a region of the phase diagram where a bicontinuous microemulsion is formed

References

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