Computational study on molecular aggregation and phase behavior in aqueous mixtures

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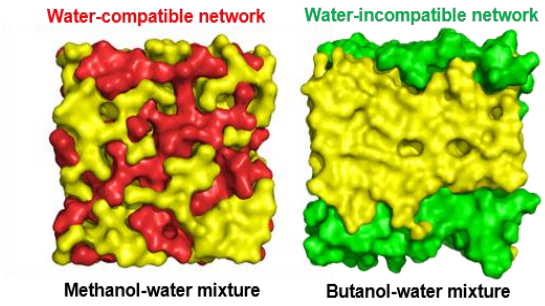
Dissolved molecules, including salt, osmolyte and alcohol affect the structure of water and the properties of aqueous solution. Solute molecules tend to be aggregated as the concentration raises. Recently, we have developed a systematic approach in combination of molecular dynamic simulation and graph theory to quantitatively describe the aggregation pattern of solute and water. [1] The two representative types of solute aggregation behavior were shown, that is, self-associating or network-forming in various aqueous mixtures. Interestingly, the self-association of solute molecules facilitates separation from liquid phase (water-incompatible), while the extended network-forming solute aggregates tend to be entangled with water H-bond network (water-compatible). This hypothesis on bifurcating aggregation pathway has been shown to contribute to establishing a relationship between molecular aggregation behavior and phase behavior such as miscibility gap, depending upon the type of ions [1], polarity of solute molecule [2], molecular shape [3], and temperature [4]. MD simulation and graph theoretical analysis in various aqueous mixtures were presented to investigate the aggregation pattern of dissolved molecules and its effect on water H-bond network.



References

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