

Thermodynamic driving force for aqueous self-assembly

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Recent molecular dynamics simulations have revealed the spontaneous formation of liquid crystals from randomly mixed binary solutions of simple solutes in water modeled using a coarse-grained potential. The liquid crystals sustain their shape through anisotropic pressure simulations, and are stable in a wide range of water-solute interaction potentials. In this work, we use molecular dynamics simulations to investigate the driving force behind the liquid crystal formation. The extent of the hydrophobic/hydrophilic interaction between the solute pair in mW water is examined at temperatures from 260 K to 340 K. The potential of mean force (PMF) of the solute pair is calculated, along with the thermodynamic signatures relating to the solute pair, including the free energy of association, enthalpy of association, and entropy of association. These calculations reveal the driving force behind the association of the solute pair, providing insight into the more complex formation of liquid crystals. Further understanding of the theoretical formation of liquid crystals may reveal candidate solutes for experimental reproduction, potentially useful in nanofluidic applications and in the experimental control of the assembly of macromolecules.

