

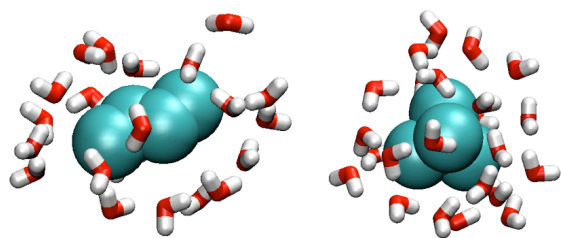
Optimized simulation model for the quantitative description of hydrophobic hydration

Outcome: A new simulation model that describes the solubility of linear and branched alkanes in water over a broad temperature range than any existing model has been developed, allowing for a more quantitative description of the hydrophobic driving forces driving self-assembly.

Impact/benefits: An accurate description of the hydrophobic effect (encapsulated by the poor solubility of oils in water and the resulting temperature dependence) is key for the predictive modeling of biomolecular association and surfactant self-assembly. Additionally, the model developed herein will find application to predicting the environmental fate of low solubility pollutants in water.

Background/explanation: To date a quantitatively accurate molecular simulation model of the solubility of alkanes in water over a range of temperatures and pressures has yet to be developed. The poor solubility of oils in water gives rise to the non-specific association of non-polar moieties that drives the collapse of polypeptide chains and association of surfactants in aqueous solution. The precise temperature dependence of this hydrophobic association is indicative of characteristic thermodynamic signatures (entropic, enthalpic, and heat capacity) that can be exploited for the triggered release of drugs from assemblies by temperature and solvent quality queues.

This was achieved by optimizing the cross solute-water interactions for a number of linear and branched alkanes over a broad temperature range to reproduce experimental solubilities using molecular dynamics simulations to determine the underlying hydration free energies. The model developed underscores the importance of accounting for missing polarization interactions, typically neglected in molecular simulations.



Caption: Butane and neopentane dissolved in aqueous solution.

Credit: Hank Ashbaugh, Tulane University.