Crustwater: An analytical statistical mechanical model to study solvation in water

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Solvation in water is one of the most important phenomena on earth as it is connected to the folding of proteins, filtration process to generate clean water, binding of a drug to its target, to name a few. However, the current modeling of solvation, within the classical approximation, suffers from drawbacks. Explicit water models in molecular dynamics simulation are computationally expensive and implicit models ignore the molecular nature of water. Recently, we have introduced, **a *fully analytical statistical mechanical model*** for solvation, termed Crustwater [1,2]. In Crustwater, pure water is treated as a collection of hydrogen bonded (h-bonded) and non-h-bonded states. The partition functions of these states are evaluated analytically and combined to generate the full partition function, from which all thermodynamic properties are calculated. To model solvation, spherical solutes are introduced in the model. Both the geometric and energetic changes, caused by the solute, are evaluated analytically to get the partition function for the solute-water system. Our solvation thermodynamics results for the inert gases and small spherical solutes show an excellent match with experiments with almost instantaneous calculation. Extension of this model for the non-spherical solutes is currently in progress. This model may eventually lead to a fully analytical model of solvation for molecules with different shapes and sizes.

Reference:

[1] Yadav, A. K.; Bandyopadhyay, P.; Urbic, T.; Dill, K. A. Analytical 2-Dimensional Model of Nonpolar and Ionic Solvation in Water. *J. Phys. Chem. B* **2021**, *125* (7), 1861–1873. https://doi.org/10.1021/acs.jpcb.0c10329

[2] Yadav, A. K.; Bandyopadhyay, P.; Coutsias, E. A.; Dill, K.A. Crustwater: Modeling hydrophobic solvation. *J. Phys. Chem. B* **2022**, *126* (32), 6052–6062. https://doi.org/10.1021/acs.jpcb.2c02695