University of Texas at San Antonio

Department of Physics & Astronomy

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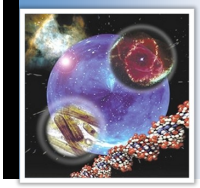
Computational Modeling of Solvent Effects

The determination of native structures of macromolecules from their primary structures and the surrounding solvent molecules and ions is of crucial importance to understand their structure-function relationship. One of the major challenge in arriving at this understanding is to elucidate the role that water molecules, ions and the primary structure play on the thermodynamic properties and conformation stability of the native structures of macromolecules. It is also of fundamental importance for this understanding to establish the impact of fragment size, mutations on the primary structure and physiological condition has in altering the conformation stability of macromolecules. This understanding would provide insight toward elucidating mayor problems such us folding process and protein structure as well as the role that surface localized water and ions plays in molecular recognition and affinity.

One major source of complexity on these phenomena arises from the strong influence the environment has on the conformational stability. Indeed, the appropriate inclusion of solvent effects on macromolecules has lead to controversial debates. In fact, predicting how salt solutions modulate the conformational stability of the native structure of macromolecules remains an unsolved challenge. In this talk, I will present the most used solvation models and I will discuss their advantages and disadvantages. I will also present a recent and promising approach that has been shown to eliminate the extremely high computational demands of full atomistic simulation calculations without loosing important structural features of complex biological activities.



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