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Models for Solvent Distributions around Biomolecules

Ions and Water Molecules have been long known to play crucial roles in governing biomolecular stability and function. Elucidating how ions and water molecules distribute themselves around the solutes should provide valuable insights in the mechanism of how those molecules function and also provide experimental tests for theoretical predictions. I will discuss the 3D-RISM integral equation approach, emphasizing tests that involve comparisons to X-ray scattering results both in solution and in crystals and to ion-counting experiments for nucleic acids.

Biography:

David A. Case has worked in the area of biochemical computer simulations for more than 40 years. He received a Ph.D. from Harvard University and has worked at the University of California, Davis, The Scripps Research Institute and Rutgers University.

Research interests include compuatational aspects of biomolecular NMR and crystallography and the development of molecular dynamics-based simulation methods. He leads the team that develops the Amber suite of biomolecular simulation programs.