

Abstract: The advent of many efficient and powerful computational methods and tools paves the way for the bright future of computational chemistry. Due to the development of modern computer simulation techniques, it is now possible to predict many structural, thermo-physical, dynamical and electronic properties of a chemical system in various environments. In this talk, my current as well as past research on some of the important chemical systems will be presented. The structural, dynamical and spectral aspects of these chemical systems will be discussed in a microscopic level. The main focus will be on topics like vibrational spectral diffusion in water as well as aqueous solutions, reactive solvation of energetic material and the development of a new class of ionic liquids containing N-heterocyclic anions for capturing carbon dioxide.