

Joint CQSE and CASTS Seminar

Weekly Seminar
Oct. 7, 2011 (Friday)

TIME Oct. 7, 14:30 ~ 15:30
TITLE Challenges in Modeling Water: Toward a first-principles based Multi-model Method
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Abstract

Water is one of the most important substances of life, but the detailed structure and dynamical properties at interfaces is far from well understood. Many fundamental questions in biology, chemistry and physics are directly related to the chemical and physical properties of interfacial water. For examples, it was noted that water's interactions with proteins play an essential role in determining the folding mechanism and the functions of the protein. The solvation of various atmospherically important chemicals at water/air interface dictates the reactivity of aerosols, which are known to affect not only short-term air pollution but also long-term climate changes. Furthermore, effects of water on the electrochemical reaction on semi-conductor and metal surfaces are larger unknown which hinder the efficiency of converting solar energy for water splitting – an important and critical issue in energy research. One of the common themes for the above-mentioned subjects is the rough energy landscape of aqueous systems that hinder a straightforward way for a structural determination from first-principle methods.

Our recent effort in developing a first-principle based multi-model methods is to integrate the efficiency of empirical models and the accuracy of first-principle methods to study various aqueous systems ranging from large-sized water clusters, water interfaces, to various condensed phases (low temperature amorphous phases and proton ordering process). For clusters, we can benchmark the commonly used DFT methods against other high-level quantum chemistry methods and in condensed phases, we also seek for comparisons with quantum Monte Carlo methods. In this talk, we will discuss some of the successes and failures we have encounter and how we utilize the information learnt to move toward a consistent picture in simulating aqueous systems.

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