Methods and Models for Condensed Phase Simulation of Water

Teresa Head-Gordon

Departments of Chemistry, Bioengineering, and Chemical and Biomolecular Engineering Chemical Sciences Division, Lawrence Berkeley National Laboratory University of California, Berkeley, CA 94720

I will discuss new theoretical models and methods that address accuracy and tractability for advanced potential energy surfaces. These models and their implementations are opening up new abilities for allowing both accuracy and larger scale simulations of complex molecular fluids, solids, and their mixtures. I will highlight some recent new ab initio simulations of meta-GGAs of liquid water and discuss their performance.