

Multi-scale Modeling of Chemistry in Water

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Molecular dynamics simulations of chemical reactions in water can be significantly accelerated by exploiting the local nature of chemical reactivity, and describing a reactive region at the quantum mechanical (QM) level, while the environment is described at the more approximate molecular mechanical (MM) level. The challenging aspect of such simulations is the diffusive nature of the solution, with water molecules that flow in and out of the reactive region. Over the past decade several QM/MM models have appeared; Constrained QM/MM models in which the QM water molecules are constrained within a reactive region, and adaptive QM/MM models in which the water molecules change description as they flow across the QM/MM boundary. These approaches have the potential to extend the impact of QM/MM far beyond the rigid (bio) systems for which it is now predominantly used. The different models have varying degrees of complexity and (inversely related) accuracy, but there is currently no one model that has been adopted as a widespread molecular modeling tool. I will discuss some of the main bottlenecks to widespread application, present our new developments on both adaptive and constrained models, and compare performances of the different approaches in describing nucleophilic addition reactions in water.