Improving the accuracy and time scales of ab initio molecular dynamics simulations for actinide and geochemical systems: Exact exchange, free energy, and parallel in time algorithms

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Abstract

Mechods of directly simulating the behavior of complex strongly interacting atomic systems (molecular dynamics, Monte Carlo) have provided important insight into the behavior of nanoparticles, biiochemical sysytems, actimide systems and geofluids. The limitation of these methods to even wider application is the difficulty of developing accurate potential interactions in these systems at the molecular level that capture their complex chemistry. Ab inito molecular dynamics methods have provided a means to simulate dynamics from molecules to large nanoscale systems. However, these methods have been limited to low level of electronic structure theory and short time-scales. This talk will focus on our developments in two areas: implementation of exact exchange, and application and development of free energy and parallel in time algorithms. The talk will focus on the fundamentals of these methods and the realities in terms of system size, computational requirements and simulation times that are required for their application. Recent applications of these methods will be shown for solvated actinide complexs and their interaction with mineral surfaces.