Quantum wavepacket ab initio molecular dynamics: Applications to vibrational properties in hydrogen-bonded clusters and hydrogen tunneling in biological enzymes

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Abstract

This talk is arranged in three parts: The first part of the talk deals with the discussion of a computational methodology developed within our group. The approach combines quantum wavepacket dynamics with ab initio molecular dynamics and is potentially useful in studying problems where nuclear quantum effects can play an important role. Computational bottlenecks and associated solutions are also discussed. The chemical applications portion of the talk will contain two portions where I will discuss applications of this approach that result in interesting insights in (a) hydrogen tunneling in biological enzymes, and (b) solvation structure, dynamics, and simulation of vibrational spectroscopy in hydrogen-bonded molecular clusters.