DAMOP14-2014-000974

Abstract for an Invited Paper
for the DAMOP14 Meeting of
the American Physical Society

Non-Born-Oppenheimer Dynamics in Ring-Opening and Biological Processes

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We discuss simulations of nonadiabatic dynamics in molecular systems, highlighting the role of conical intersections. The influence of conical intersection shape and energy is explored. We summarize new methods for calculating the electronic structure and dynamics on graphical processing units, which are leveraged in order to enable simulation of excited state molecular dynamics in systems containing hundreds of atoms. Specific systems studied encompass photoinduced isomerization about carbon double bonds and ring-opening reactions. We discuss the basic mechanisms of these processes in isolated molecules, including direct comparison of theoretical and experimental results. We further discuss the role of solvent and/or protein environments in directing and modifying these processes.