Ab Initio Molecular Dynamics on Excited Electronic States

Todd J. Martínez
Department of Chemistry, Stanford University, Stanford, CA 94305
and
SLAC National Accelerator Laboratory, Menlo Park, CA 94025

Abstract: We discuss recent progress in nonadiabatic ab initio molecular dynamics. We summarize improvements in the dynamics methodology, specifically focusing on ab initio multiple spawning techniques. We also discuss new approaches to the electronic structure problem which can accelerate this sufficiently for use in ab initio molecular dynamics. These approaches include tensor hypercontraction formalisms, the development of new algorithms for graphical processing units, and ab initio exciton models that can treat dynamics in large multichromophoric photosynthetic molecules containing up to 4000 atoms.