Potential Energy Surfaces and Nonadiabatic Dynamics in Photoactive Proteins from First Principles

Todd J. Martínez[a,b]

a Department of Chemistry and The PULSE Institute, Stanford University, Stanford, CA 94305, b SLAC National Accelerator Laboratory, Menlo Park, CA 94025
toddjmartinez@gmail.com

We discuss new efficient and accurate approaches for the computation of excitation energies and nonadiabatic dynamics in proteins, including both static and dynamic electron correlation. A graphical processing unit (GPU)-based implementation of the tensor hypercontracted XMS-CASPT2 method is described, enabling computations of excitation energies for hundreds of quantum mechanically-treated atoms (and further including thousands to tens of thousands of surrounding atoms treated by an empirical force field).[1,2] We also describe our GPU-based implementation of the state-interaction/state-averaged restricted ensemble Kohn-Sham (SI-SA-REKS) method.[3,4] We compare the performance and accuracy of this method to conventional XMS-CASPT2 and show that SI-SA-REKS can provide XMS-CASPT2 accuracy at a cost which is nearly that of ground state DFT. We apply the SI-SA-REKS method in combination with ab initio multiple spawning to the nonadiabatic dynamics of channelrhodopsin-2,[5,6] a protein which has seen wide use in optogenetics.

References
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