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

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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).\textsuperscript{1,2} We also describe our GPU-based implementation of the state-interaction/state-averaged restricted ensemble Kohn-Sham (SI-SA-REKS) method.\textsuperscript{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 \textit{ab initio} multiple spawning to the nonadiabatic dynamics of channelrhodopsin-2,\textsuperscript{5,6} a protein which has seen wide use in optogenetics.

References