Nonadiabatic processes in condensed phase systems with ΔSCF

Momir Mališ, Eva Vandaele, Sandra Luber

Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zürich, Switzerland
momir.malis@uzh.ch

The variational delta self-consistent field (ΔSCF) density functional theory (DFT) based method enables full atomistic simulations of nonadiabatic processes in condensed phase systems by balancing computational costs and accuracy of the description of excited electronic state properties. This avoids the bottleneck of computing all the excited electronic states in the usually dense excited electronic state manifolds encountered during the nonadiabatic molecular dynamics in the condensed phase, for example with time-dependent DFT methods, but instead only the excited electronic states of interest are directly determined. We will discuss novel Ansätze in order to incorporate spin-orbit coupling and certain multi-reference characters into ΔSCF calculations. We applied our methodology for the investigation of nonradiative deactivation mechanisms in a number of solvated systems, emphasizing the details of chromophore-environment interactions and their influence on photochemical processes in condensed phase systems.

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