MAR15-2014-008799

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Multi-reference vs. single-reference quantum chemical methods in surface hopping dynamics

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The reliability of quantum chemical methods plays a critical role in performing reliable nonadiabatic dynamics simulations. Unfortunately, the methods for computing excited states including larger regions of the energy surfaces are still computationally expensive or need support from higher level methods. In this talk the capabilities of multireference (MR) versus single reference (SR) methods will be discussed. In terms of SR approaches we focus our attention on the second-order algebraic diagrammatic construction method (ADC(2)). In addition to the direct calculation of nonadiabatic coupling vectors also the method of computing wavefunction overlaps between consecutive time steps is used. Several interesting examples are discussed such as the charge transfer between π systems and the photodecativation of adenine. In the latter example an extensive comparison of the results concerning deactivation pathways and decay times is given for different methods including multireference configuration interaction, ADC(2) and time-dependent density functional theory (TDDFT) using various functionals. The surface hopping dynamics simulations are performed on the basis of the public domain program system NEWTON-X [M. Barbatti, M. Ruckenbauer, F. Plasser, J. Pittner, G. Granucci, M. Persico, and H. Lischka, WIREs:CMS 2014, 4, 26-33].