This is the way: Excited state simulations using SHARC

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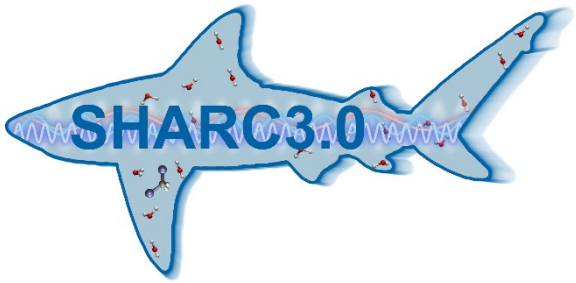
Want to do non-adiabatic excited state dynamics? SHARC is the way! SHARC is a suite created at the University of Vienna to perform excited state simulations. SHARC stands for Surface Hopping including ARbitrary Couplings [1]. This means that the nuclei move according to classical trajectories on the potential energy surface of one particular electronic state and hop to another potential by means of a stochastic algorithm. In order to determine when a hop takes place, SHARC can include any arbitrary coupling, typically non-adiabatic couplings and spin-orbit couplings, but also dipole couplings to describe the interaction of molecules with laser fields. The latest version of the code, SHARC3.0, has been released in April 2023[2] and besides surface-hopping includes Ehrenfest simulations developed at the University of Minnesota. SHARC is currently interfaced to many electronic structure codes to enable on-the-fly quantum chemistry at many different levels of theory. Additionally, it is possible to use underlying neural network potentials [3], vibronic coupling models [4], or be combined with sampling methods in the excited states [5], pushing simulations times from typically sub-ps to ns or longer. The inclusion of explicit environment is possible using hybrid quantum mechanics/molecular mechanics (QM/MM) models, e.g. using COBRAMM [6]. Besides introducing the code and its capabilities, I will illustrate the broad applicability of the code with several examples of excited state simulations in organic molecules and transition metal complexes, in gas phase, solution or a biological environment.



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