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Excited-state dynamics using the SHARC4 package

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Nonadiabatic dynamics simulations in the excited electronic states are nowadays essential for research in spectroscopy, photochemistry and -biology, and materials science. One of the most widely used nonadiabatic dynamics methods is trajectory surface hopping, which is the core method implemented in the SHARC (Surface Hopping including ARbitrary Couplings) package. The recent updates to versions 4.0 and 4.1 include a wide array of new methodological options. Most importantly, the new hierarchical electronic structure interface framework [1] enables multiscale modeling of extended systems via QM/MM and LVC/MM [2], the description of multi-chromophoric systems [3], the sampling of excited-state free energy surfaces [4], automated machine learning training [1], the modeling of the excitation process with realistic laser pulses [5], and many other possibilities. In my talk, I will provide an overview of the SHARC4 package and its methods and show corresponding applications.

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