Excited-state nonadiabatic dynamics in explicit solvent using machine learned interatomic potentials

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Simulating complex systems containing thousands to millions of atoms remains a major challenge in computational chemistry, particularly for excited-state dynamics, where classical force fields fail to capture quantum effects. The Quantum Mechanics/Molecular Mechanics (QM/MM) approach has been widely used to study such systems, but it suffers from the inherent computational cost and poor scaling of quantum mechanical methods.

Recent advancements in machine-learned interatomic potentials offer a promising alternative by replacing the quantum mechanical treatment in QM/MM simulations, significantly accelerating calculations. One such model, FieldSchNet[1], incorporates the electric field generated by MM atoms to capture electrostatic interactions between the different regions, mimicking the electrostatic embedding in a QM/MM description. In this work, we apply FieldSchNet to excited-state surface hopping dynamics. Using nonadiabatic QM/MM simulations of furan in water, we generate training data for the five lowest singlet states and assess the performance of different training and testing strategies in reproducing the original dynamics.

[1] M. Gastegger, K. T. Schütt and K.-R. Müller, *Chem. Sci.*, **2021**, *12*, 11473-11483.