

Abstract

Nonadiabatic molecular dynamics is an important approach for the study of photochemical phenomena. Using a stochastic algorithm and a set of trajectories, it is possible to study phenomena where the Born-Oppenheimer approximation breaks down. This approach is limited by the size of the molecule and the length of time intervals that can be studied. Machine learning techniques, which have proven themselves in many different fields, can be a helpful tool. In this thesis, I focus on the applicability of a kernel ridge regression technique as a potential tool for accelerating nonadiabatic molecular dynamics simulations. Vinyl bromide is a small molecule with a heavy bromine atom, which from a computational point of view represents a suitable test system for nonadiabatic molecular dynamics with the inclusion of non-adiabatic and spinorbital couplings.