

# ABSTRACT

## Ab initio molecular dynamics with non-adiabatic and spin-orbit effects applied to time-dependent fluorescence

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Fluorescent probes are essential for many experimental techniques in biochemistry and microbiology. Accurate simulations of these molecules are theoretically challenging as they can involve conical intersections and intersystem crossings as well as interactions with the environment.

This thesis is a compilation of papers dealing with development, implementation, and application of ab initio molecular dynamics techniques with non-adiabatic and spin-orbit interactions that can be used to model fluorescent probes not only in the gas phase but also in the complex molecular environment of biomembranes.

Initial work involves a study of 9H-adenine using ab initio MD with non-adiabatic effect using time-dependent density functional theory and two single reference methods CC2 and ADC(2). The central part of the thesis discusses the implementation of spin-orbit coupling into surface hopping dynamics with application to deactivation of thiophene and selenophene. Further applications include studying spectra and dynamics of the fluorescence probe Prodan in the gas phase and in solution, and simulation of absorption spectra of Laurdan in biomembranes. Other systems are being investigated and will be published soon. My implementation has become a part of the official Newton-X program package.