Abstract

Extremely fast relaxation processes in photosynthetic molecular complexes and in chlorophyll molecules have been observed for decades. The emergence of multidimensional spectroscopic techniques with femtosecond temporal resolution resulted in the discovery of many new, previously unseen physical phenomena. These ultrafast phenomena (occurring on the timescale of 10^{-15} s) have been the subject of intense discussions and experimental measurements, but theoretical models of these processes are sparse. In this thesis, a new spectroscopic theoretical model for chlorophyll-like molecules is formulated and tested. The physical parameters of the model were optimised on experimental linear absorption spectra obtained from literature. The parameterised model was then used to reproduce the experimental data with great precision, and also to simulate excited state population dynamics using the Redfield equations which were derived, implemented and computationally optimised. The relaxation times of the $Q_x - Q_y$ transition in chlorophyll *a* molecule were roughly estimated from the dynamics and compared with the literature. The limitations of the new model were proposed and discussed as well.