Abstract

The photosynthetic reaction centres have uppermost importance in photosynthesis. They represent the actual place where the energy carried by photons is turned into charge-separated states which then enable to establish the electrochemical H^+ transmembrane gradient used by ATP synthases. The photosynthetic light-harvesting complexes gather the energy of light radiation and direct it in the form of electronic excitation energy into the reaction centres. The efficiency of this process is exceptionally high, close to unity, what is capturing the interest of researchers for decades. The development of experimental techniques has led to better understanding of this process down to atomic scale. Nowadays, this insight along with the theoretical basis stemming from quantum mechanics can be used to perform accurate computer simulations which can determine properties of the whole molecular aggregates independently of experiments. This thesis provides an introduction into the field of theoretical photosynthesis research, and it summarises the progress made in past two decades. The detailed theoretical approaches are being put into perspective of the reaction centres of photosynthetic purple bacterium *Rhodobacter sphaeroides* which is a valuable model organism. Both experimental and theoretical results of excitation energy transfer times are compared on this model example.