In this thesis the electron hopping of selected heterocyclic compounds and selected carotenoids was studied using QM/MM simulations of excited states dynamics. Tully electron hopping and semiempirical methods OMx in combination with MRCI method was used in the simulations. Calculations were performed using Newton-X, MNDO99, MNDO2020 and Gromacs. The lifetimes of the excited states were estimated based on the simulations. The results showed that used methods correctly describes the time evolution of excited states of heterocyclic compounds. In case of carotenoids only deexcitation from first excited state was described correctly.