Title: Quantum mechanical study of the electron hoping processes of pigments from photosystems. Simulation of absorption and emission photoelectron spectra.

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Abstract: The aim of this thesis is to develop a methodology for simulation of dynamical properties of carotenoids by OMx method combined with surface electron hopping. We use linear conjugated polyenes: ethene, butadiene, hexatriene up to polyenes with 22 carbon atoms as model systems. First, the spectra are calculated with sufficiently good agreement with the experimental data by both correct order of excited states and small deviation from experimental data. These results are used for electron surface hopping for calculation of mean lifetimes of excited states of studied polyenes. Calculated lifetimes are of the same order as experimental data for butadiene, hexatriene and octatetraene. Calculated lifetimes for poleynes with 20 resp. 22 carbon atoms agree well with chemically analogous carotenoids.

Keywords: quantum mechanics, photoelectron spectra, pigments of photosystems, elecrton transitions, molecular and electronic dynamics