Abstract

We present an improved model of charge carrier photogeneration in π-conjugated polymers with weak intermolecular interactions based on the model of Arkhipov. It includes quantum effects affecting the creation of charge transfer states, which occurs as an intermediate step in the free charge carrier photogeneration process. The electrostatic potential between the electron and the hole and transfer integrals needed for the calculation of the potential barrier for the charge transfer state dissociation are calculated quantum-chemically. We apply our model on experimental data of the charge carrier photogeneration efficiency in poly[1-trimethylsilylphenyl,2-phenyl]acetylene to explain its dependence on applied electric field. We eliminate several problems of the previous model. We are able to fit experimental data with just one set of parameters in the whole interval of the applied electric field. We do not have to consider several intervals of the electric field separately as in the previous work and reduce the number of needed parameters to three.