In the last years, we have developed a computational methodology to simulate charge transfer processes in complex systems. Due to the large system size, which has to be treated quantum mechanically, we have developed a coarse-grained quantum/classical methodology, which allows to describe the dynamics of the electronic system coupled to the dynamics of environment, e.g. the protein in water solvent. Charge-transfer (CT) parameters are computed using a fragment orbital approach applying the approximate Density Functional method SCC-DFTB. Environmental effects are captured using a combined quantum mechanics/molecular mechanics (QM/MM) coupling scheme and dynamical effects are included by evaluating these CT parameters along extensive classical molecular dynamics (MD) simulations. Using this methodology, the time course of the charge can be followed by propagating the hole wave function using the time dependent Schrödinger equation for the Tight Binding Hamiltonian, which can also be used to compute the transmission and current through e.g. DNA nano-wires. The photo-activation of E. coli Photolyase involves, after photoexcitation of the chromophore and energy transfer to FAD, a long range hole transfer along a chain of Trp residues. Since this process could not be modelled using Marcus theory with parameters computed with classical equilibrium MD simulations, we used fully coupled non-adiabatic (Ehrenfest/surface hopping) quantum mechanics/molecular mechanics (QM/MM) simulations. The most recent extension concerns applications to charge and exciton dynamics in organic materials,

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