Quantum Efficiency Seminar und Colloquium

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Simulation of charge transfer in complex systems: Merging model Hamitonian approaches with electronic structure calculations and classical molecular dynamics simulations

In the last years, we have developed a computational methodology to simulate charge transfer processes in complex systems. First applications were concerned with charge transfer in DNA, which has received much attention in the last years due to its role in oxidative damage and repair in DNA, but also due to possible applications of DNA in nano-electronics. Currently, we are extending and applying the methodology to study CT in organic materials.

Charge-transfer (CT) parameters are computed using a fragment orbital approach applying the approximate Density Functional method SCC-DFTB (1,2). 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 hole can be followed by propagating the hole wave function using the time dependent Schrödinger equation for the Tight Binding Hamiltonian (5,6), which can also be used to compute the transmission and current through DNA nano-wires with the Landauer formalism.

6. B. Popescu et al., Time-Dependent View of Sequential Transport through Molecules with Rapidly Fluctuating Bridges, PRL 109 (2012) 17680