Physikalisches Institut
Fakultät für Mathematik und Physik
Albert-Ludwigs-Universität Freiburg

QE

Quantum Efficiency Seminar und Colloquium

MARCUS ELSTNER

Karlsruhe Institute of Technology

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.

1. T. Kubar, P. Woiczikowski, G. Cuniberti, M. Elstner, Efficient Calculation of Charge-Transfer Matrix Elements for Hole Transfer in DNA, J. Phys. Chem. B, 112, (2008) 7937.

2. T. Kubar, M. Elstner, What governs the charge transfer in DNA? The role of DNA conformation and environment. J. Phys. Chem. B, 112, (2008) 8788

3. P. Woiczikowski, T. Kubar , R. Gutierrez, R. Caetano, G. Cuniberti, M. Elstner, Combined DFT and Landauer approach for hole transfer along classical MD simulations of DNA, J. Chem. Phys. 130 (2009) 215104.

4. T. Kubar, U. Kleinekathoefer, M. Elstner, Water Drives the Hole Transfer in DNA: a Combined TD-DFT and Classical MD Study, J. Phys. Chem B, 113 (2009) 13107.

5. T. Kubar, M. Elstner, Coarse-grained time-dependent density functional simulation of charge transfer in complex systems: application to hole transfer in DNA, J. Phys. Chem. B 114 (2010) 11221.

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

Date: **Tuesday, December 18th, 2012 15:45**
Location: **Lecture Hall 1, Hermann-Herder-Str. 3, Freiburg**

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