# *A coarse grained QM/MM approach for the description of hole transfer in DNA*

Marcus Elstner, Karlsruhe Institute of Technology (Germany)

Charge transfer in DNA 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. Despite intense experimental and theoretical efforts, the mechanism underlying long range hole transport is still unresolved. This is in particular due to the fact, that charge transfer sensitively depends on the complex structure and dynamics of DNA and the interaction with the solvent environment, which could not be addressed adequately in the modeling approaches up to now. We present a new computational strategy to evaluate the charge-transfer (CT) parameters for hole transfer in DNA. Based on a fragment orbital approach, site energies and coupling integrals for a coarse grained tight binding description of the electronic structure of DNA can be rapidly calculated using 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. This methodology allows to analyze in detail several factors responsible for CT in DNA. The fluctuations of the counterions, strongly counterbalanced by the surrounding water, leads to large fluctuations of the site energies, which govern the hole propagation along the DNA strand, while the electronic couplings depend strongly on DNA conformation and are not affected by the solvent (2) . 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 coarse grained Hamiltonian (5,6).

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