The Multi-Scale Dynamic Model of Charge Transport through DNA Structures

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A new computational model using a hybrid quantum-classical approach for the simulation of charge transfer through DNA has been developed and applied to understand the effect of thermal fluctuations on charge transport rates. The model also allows us to study charge transfer during dynamic processes, such as DNA melting and stretching. Molecular dynamics simulations with the empirical AMBER forcefield provide a set of geometrical configurations of the DNA bases. Quantum mechanical calculations (using ZINDO) are then used to calculate the electronic coupling and thermodynamic driving force for charge transfer between all pairs of consecutive bases for many molecular conformations. These quantities are used to calculate charge transfer rates between each stacked base pair from the Marcus equation. A newly developed method of stochastic time evolution of charge within DNA is then used to calculate the overall transport rates along the DNA dodecamer (5′-CAAAAAAAAAGC-3′). The model assumes that charge transfer occurs by way of a simple hopping mechanism.