

LONG-RANGE CHARGE TRANSFER IN DNA

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A quantum-mechanical model of a charge transfer in a multi-site system has been considered applying for DNA fragment, where a Watson-Crick base pair corresponds to each site. The corresponding system of nonlinear differential equations was numerically solved by the Runge-Cutta method of the fourth order of accuracy with a constant step. This method appears to be quite appropriate in calculations at large periods of time.

We examined the 200-site chains consisting of identical sites at different values of the parameters. Typical patterns of transfer, involving the possibilities of superexchange and hopping transfer, as well as transfer through excitations of polaron and soliton types, have been obtained from a large number of numerical experiments made.

Also we examined the 150-, 200- and 250-site chains with donor and acceptor. In modeling the donor we decreased the electron energy at the sites. For the acceptor we increased frequencies and friction coefficients for classical subsystem and decreased the electron energy at the sites. Calculations were made for different meanings of the parameters. Though the time of irreversible charge transfer may differ ten-folds for different values of the donor and acceptor parameters, the qualitative picture of excitation transfer remains similar. The excitation arises at the "locus of formation", migrates along the polynucleotide chain. After several reflections it virtually "smears" uniformly over the entire chain and remains in this state for rather a long time. Then the probability of charge localization at the acceptor starts increasing and gradually becomes close to 1.

On the basis of the results of a large number of computer experiments the following can be assumed. Transfer occurs, if the energy electron values at the donor and at the acceptor are close to the those at the bridge sites. There is an "optimal depth" of the acceptor site well, for which transfer time will be the shortest. The transfer time decreases when the frequency and friction coefficients at the acceptor sites increase, while the frequency values are sufficiently near the values of matrix elements. The transfer time depends on initial conditions - it is the shortest if the excitation is localized at the start moment on the first site, and it is maximal when probability is uniformly distributed over the all donor sites. The time during which the trapped state is formed, i.e. the time of transfer, has shallow dependence on the transfer distance and is almost entirely determined by the acceptor parameters and the initial state at the donor. The numerical experiments have demonstrated that the electron density can be trapped by "trap sites" even if the number of such sites is 1, but then it must not be localized just at the end; after this site it is necessary to add a number of "middle chain sites", large enough for a polaron state to form at the end of the chain. Another condition necessary for the trapping to take place is the availability of a potential well whose depth is equal (in the order of magnitude) to the oscillation energy of the "trap sites".

These results are in good agreement with the views on the energy control over the transfer rate, which hold that the energy characteristics of the donor, the bridge and the acceptor should be correlated and close in the values.