Contribution ID: **273** Type: **Sectional reports**

Direct Simulation of the Charge Transfer along Oligonucleotides at T=300K

Friday, 14 September 2018 10:30 (15 minutes)

At present, the attention of researchers is attracted to the possible mechanisms of charge transfer in quasy-1D biomacromolecules, such as DNA, in connection with the potential use of this nano-objects in nanobioelectronics.
Biophysical experiments on the hole transfer from guanine G (donor) to guanine triplet GGG (acceptor), separated by adenine-thymine (A-T) bridges of various lengths, demonstrate that the rate of charge transfer between donor and acceptor decreases exponentially with increasing separation only if the guanines are separated by no more than three base pairs; if more bridging base pairs are present, the transfer rates exhibit only a weak distance dependence.
We performed direct numerical experiment on the charge transfer from donor to the acceptor along bridge, consisting of homogeneous sites. The model is based on the semi-classical Holstein Hamiltonian. The Holstein polaron model is simple but relevant for explaining charge transfer in DNA. To take into account the temperature, Langevin thermostat is used.
For computation we chose some parameter values as for DNA model: the charge donor is guanine G, acceptor - guanine triplet GGG, and the bridge consists of adenines A or thimines T with number of sites N. We modeled different length of bridge N from 1 to 26 sites (length of the whole chain is from 5 to 30 sites).
For each N we calculated a set of 100 samples at temperature 300 K, and estimated time-dependencies averaged over the ensemble. The sample is a trajectory of system with its own initial data and pseudorandom time series, which modeling medium thermal fluctuations. Initial data for classical sites are chosen from Maxwell distribution corresponding to T = 300 K, and the charge at moment t = 0 is localized on the donor. We calculate the samples until the probabilities of charge distribution on the sites become similar to the thermodynamic equilibrium state, and estimate the time t_TDE to reach this state.
Results of the simulation demonstrate that: for short chains (N<4 for bridges of adenines and N<5 for thymine bridges) the value of t_TDE increases exponentially with the increasing N; for big N, t_TDE values are almost the same. In suggestion that the charge transfer rate is a reciprocal of the time t_TDE, the results of computer modeling and data of biophysical experiments have a qualitative similarity.
We are grateful to the HybriLIT group of JINR for computational resources. The work is partially supported by the Russian Foundation for Basic Research, projects no. 16-07-00305, 17-07-00801,
and Russian Science Foundation, grant 16-11-10163.

Primary author: Dr FIALKO, Nadezhda (IMPB RAS - the Branch of KIAM RAS)

Co-author: Prof. LAKHNO, Victor (IMPB RAS –the Branch of KIAM RAS)

Presenter: Dr FIALKO, Nadezhda (IMPB RAS - the Branch of KIAM RAS)

Session Classification: 12. Bioinformatics

Track Classification: 12. Bioinformatics