## International Conference "Mathematical Modeling and Computational Physics, 2017" (MMCP2017)



Contribution ID: 59

Type: not specified

## Modeling of charge dynamics in homogeneous chain with defect

Tuesday, 4 July 2017 14:45 (15 minutes)

Various results of numerous biophysical experiments on charge transfer along DNA fragment have demonstrated that different transport mechanisms are possible in DNA. The transfer rate depends not only on the length of the chain along which the transfer occurs, but also on its sequence [1].

We have studied the simple 1*D*-model based on the semi-classical Holstein Hamiltonian for a discrete chain of sites (for DNA sequence, the site is a complementary base pair) with temperature T (Langevin-type equations). Recently, using the computer simulation, it has been shown that the charge distribution in homogeneous chains in thermodynamic equilibrium (TDE) depends not only on the temperature, but also on the length of the chain.

When the energy of the classical chain  $Ecl = Nk_BT$  (N is the length of the chain) is less than the critical value *E*, *the charge is in the polaron state. When Ecl > E*, the charge is in a delocalized state [2].

For homogeneous DNA fragments, in TDE the polaron state exists at low temperatures, less than 5 Debye temperature, below which the semiclassical approximation is inapplicable. We have investigated the TDE states in the case when a trap-site with negative electron energy is placed in the middle of a homogeneous chain. Computational experiments were carried out for parameters corresponding to polyA fragments.

A qualitative picture of the total energy E, averaged by set of samples, for homogeneous chain with a trap is the same as for the chain without defect. The temperature stability of polarons in a chain with trap-site increases in comparison with the case of a homogeneous chain. For oligonucleotide AAAAGAAAAA (N = 10), the critical temperature  $T \sim E/N \sim 400$  K is in the region of biological temperatures, and for the 40-site chain of adenine with guanine in the center  $T^* < 175$  K.

The simulation results demonstrate that as the length of the chain increases, the type of charge distribution changes. In short chains, the charge is in the polaron state, and its transfer occurs slowly by hopping mechanism [3]. In long chains at the same temperature, the charge is in delocalized state, and the transfer process is more rapid.

This work is partially supported by Russian Foundation for Basic Research, grants no. 16-07-00395, 17-07-00801, and Russian Science Foundation, project 16-11-10163.

## Short biography note

[1] H.-A.Wagenknecht (ed.). Charge Transfer in DNA: From Mechanism to Application. Wiley, 2006.

[2] N.S. Fialko, E.V. Sobolev, and V.D. Lakhno. On the calculation of thermodynamic quantities in the Holstein model for homogeneous polynucleotides. JETP 123 (4), 635, 2017.

[3] M. Bixon, J. Jortner. Energetic control and kinetics of hole migration in DNA. J.Phys.Chem. B 104 (16), 3906, 2000.

**Primary author:** Dr FIALKO, Nadezhda (Institute of Mathematical Problems of Biology RAS – the Branch of Keldysh Institute of Applied Mathematics of Russian Academy of Sciences)

**Co-authors:** Dr PYATKOV, Maxim (IMPB RAS - Branch of KIAM RAS); Prof. LAKHNO, Victor (IMPB RAS - Branch of KIAM RAS)

**Presenter:** Dr FIALKO, Nadezhda (Institute of Mathematical Problems of Biology RAS – the Branch of Keldysh Institute of Applied Mathematics of Russian Academy of Sciences)

Session Classification: Bioinformatics and computational biophysics (I)