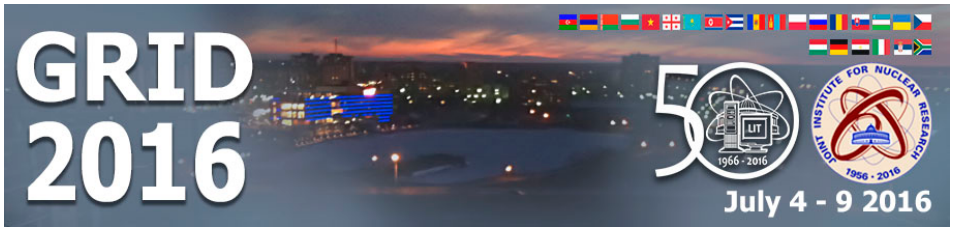

Contribution ID: **57** Type: **Plenary reports**

Modeling of electron dynamics and thermodynamics in DNA chains

Friday, 8 July 2016 09:20 (20 minutes)

The lecture gives a review of numerical experiments on a charge transfer in DNA. The charge motion is described in terms of quantum mechanics, whereas vibrational degreese of fredom are treated both classically and quantum mechanically. Special attention is given to dynamics of polaron state formation, polaron motion in electric field, Bloch oscillations and breather states.
The dynamics of charge migration was modeled to calculate temperature dependencies of its thermodynamic equilibrium values such as energy and electronic heat capacity in homogeneous polynucleotide chains.
The work was done with partial support from RFBR, project № 16-07-00305 and RSF project № 16-11-10163.
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