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Modeling of electron dynamics and thermodynamics in DNA chains

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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 degrees of freedom 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.

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References

1. A.P.Chetvericov, W. Ebeling, V. Lakhno, A.S.Shigaev, M.G.Velarde, Eur. Phys. J.B., (2016) 89:101
2. N. Fialko, E.Sobolev, V. Lakhno, Phys. Lett. A, (2016), 380, 1547
3. Lakhno V.D., Fialko N.S. Math. Biol. Bioinf, (2015), 10(2), 562

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