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Electronic, Dynamical and Thermodynamic Properties of DNA

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The idea to use DNA molecule as a base element for nanobioelectronics is discussed.

It could be considered as some molecular wire where a typical charge transfer/transport pattern can physically be viewed as a polaron and/or soliton which mobility can be very low.

A computer experiment demonstrates that mobile breather excited near one of the ends of DNA can trap the polarons. The formed quasiparticle can move along the molecule for a long distance and does not require the electric field.

The dynamics of charge migration was modeled to calculate temperature dependencies of its thermodynamic equilibrium values such as energy, electronic heat capacity and reaction constants for different nucleotide sequences. The mechanism of charge transfer for a long distance due to polaron melting is considered.

Special attention is given to: dynamical behavior of electrons in regular polynucleotide chains, dynamics of polaron states formation in Peyrard –Bishop-

Dauxois chain, polaron motion in an electric field, the role of dispersion, Bloch oscillations and breather states.

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