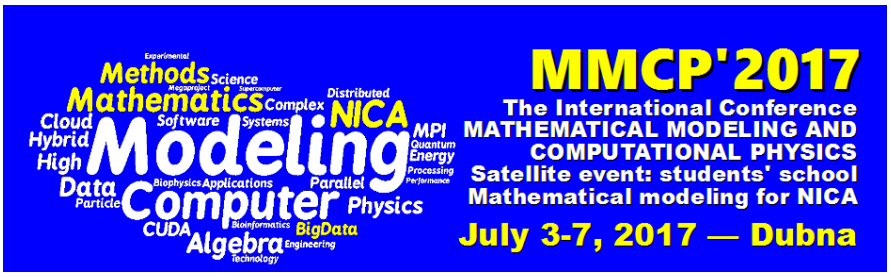

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Dynamical and Thermodynamic Electronic Properties of DNA

Tuesday, 4 July 2017 08:30 (30 minutes)

Dynamical properties of electron motion in molecular chains are considered. The charge motion is described in terms of quantum mechanics, whereas vibrational degrees-of-freedom are treated both classically and quantum mechanically.
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 adenine fragments. The peak on the graph of electronic heat capacity is observed at the polaron decay temperature.
A typical charge transfer/transport pattern can physically be viewed as a polaron and/or soliton. A closed analytical expression for charge carrier velocity dependence on electric field has been derived and analyzed in detail.
Special attention is given to: dynamical behavior of electrons in rigid chains, band structure of regular polynucleotide chains, dynamics of polaron states formation in Holstein chain, polaron motion in an electric field, the role of dispersion, Bloch oscillations and breather states.
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