Polaronic transport through DNA molecule

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Here we present the theoretical studies of sequential quantum transport of virtual polarons through DNA-based junction. For the sake of simplicity, we analyze poly(dG)-poly(dC) DNA molecule which is treated as a linear chain of quantum dots, where only one HOMO level on each GC pair is taken into consideration, while the coupling with the electrodes is described within a broad-band theory. Since the residence time of the charge carrier on the guanine G (nucleobase with lower oxidation potential) is long in comparison with characteristic time associated with molecular vibrations, the hole-type (positive ion) transport is treated as incoherent process. Decoherence itself is modeled trough the use of complex dephasing potential. Since GC bases involved into the conduction process are thermally activated to vibrations (phonon modes are excited) and vibrational coupling parameter is sufficiently strong, charge carriers are locally coupled to phonons, leading to polaron formation.

Nonperturbative computational scheme, used in this work, is based on Green's functions theory within the framework of the so-called polaron transformation (GFT-PT) [1]. This method maps exactly the many-body hole-phonon interaction problem into a one-body multi-channel scattering problem, where the availability of particular pseudo-channels is determined by an appropriate weight factor. In particular, the strong temperature-dependence of the linear conductance and nonlinear current flowing through short poly(dG)-poly(dC) DNA molecule is discussed in detail and compared to some experimental results [2].

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[1] K. Walczak, J. Magn. Magn. Mater. (2006) and Physica E (2006), both in press.
[2] K.-H. Yoo *et al*., Phys. Rev. Lett. **87** (2001) 198102.

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