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Nanoelectronic of DNA-based segments with a diluted base pairing topology

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We report in this work a quantum-mechanical investigation of the one-electron states in DNA-based segments with a diluted base pairing topology. Our main intention was to reinforce that the resonance mechanism reported in our work leads to an anomalous wave-packet dynamics, even in the worse case of strong localization in single-strand molecules. Specifically, we will consider poly(CG) and poly(CT) segments in a special topological case in which the guanine (G) bases are attached laterally at a fraction of the cytosine (C) bases. Our theoretical model is based on a tight-binding electronic Hamiltonian to compute the density of states and eigen functions of the one-electron states. We will show that the model Hamiltonian for this system can be mapped onto that of the Anderson chain with diluted disorder. We will explore the influence of the effective disorder on the nature of the one-electron states as well as on the wave-packet dynamics. In particular, we will show that in segments formed with complementary units [as in poly(CG)], dilution indeed leads to a complete exponential localization of all one-electron states. On the other hand, in chains with non-complementary units [as in poly(CT)], a resonant state is not affected by the disorder and remains extended. In the presence of such resonant state, the wave-packet develops a diffusive dynamics.

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