Correlation effects in DNA: From local band insulators to local charge and spin density-wave insulators

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A ladder model which allows for a single frontier molecular orbital at each nucleoside represented by a ladder site is analyzed for DNA. It incorporates the onsite term corresponding to orbital eigenenergy contribution, the nearest-neighbor hopping term and the long range Coulomb interaction also including the crucial onsite Hubbard term. Parameter values are deduced from results of quantum chemical analyses published by different authors and based on the density functional and hybrid valence bond/Hartree-Fock approaches. The relative positions of eigenenergies for the highest occupied molecular orbitals (HOMOs) and for the lowest occupied molecular orbitals (LUMOs) of four different nucleosides containing four different bases, which are guanine (G), cytosine (C), adenine (A) and thymine (T), determine whether LUMO is the frontier orbital, which takes place when those eigenergies have relatively low values or whether HOMO is the frontier orbital, which takes place when those eigenergies have relatively high values. By using this principle, it is deduced that for base pairs G-C and A-T, stacks of which form DNA, one frontier orbital corresponds to HOMO, which is the case for for G and A, and one to LUMO, which takes place for A and T. Since the energy scale of the Coulomb interaction is highest, that interaction determines the form of the groundstate and of low lying excited states. In an approach used in the analysis and based on this observation, the terms in the Hamiltonian related with hopping are treated as a perturbation, and a unitary transformation of the initial Hamiltonian is performed, which leads to an effective Hamiltonian for the low energy sector. This task is performed for different DNA stacks of limited length by means of some computer algebra. Open and periodic boundary conditions are used alternatively in order to get some information relevant to real systems. The dependence of the results on the value of the screening length is also analyzed. It is concluded that DNA segments in which frontier orbitals in a single strand correspond to HOMO states are conventional band insulators, widely discussed in the literature devoted to transport in DNA, while segments in which frontier orbitals in a single strand correspond to staggered sequences of HOMO states and LUMO states favor charge ordering which takes the form of staggered sequences of excitations corresponding to single electrons in LUMO states and single holes in HOMO states. Virtual processes involving some high energy states induce magnetic superexchange interactions between uncompensated spins of electrons and holes. Depending on the explicit DNA-stack form, the low energy physics of charge ordered DNA segments can be described in terms of models for spin 1/2 ladders or chains.