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Resonant and non-resonant transfers of Frenkel excitons in Helical DNA-like regular structures

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Abstract. Frenkel excitons (FEs) as collectivized electronic excitations are studied using the models of two-strands regular structures with B-DNA geometry. As basic excitations we consider the excitations of the pairs of complementary bases, not the excitations of separate bases, because of the following reasons: 1. Permanent pairing of complementary bases A-T and C-G; 2. Small inter-bases distances. The following cases are treated:
A. Resonant transfer of FEs between equal pairs of complementary bases, e.g. A-T. The models of homopolymers are supposed to contain the equal pair at each step of double helix and one strand contains one base (A-A-A- ...) or alternatively ordered bases (A-T-A-T-⋯).
B. Non resonant transfer of FEs between different pairs AT↔CG. Two models are studied: a) two-step order sequence with bases in one strand A-C-A-C⋯; b) four-step order sequence in one strand A-C-T-G-A-C-⋯
The studied FEs originate from electronic excitations of the pair with transition electric dipole moment perpendicular to the helical axis (for π-π*transitions) or parallel to the axis (for n-*π transitions).
The corresponding Hamiltonians for each case allow to calculate the tensors of dielectric permittivity and gyration tensors, by using Green functions method (at temperature T=0). The calculations give formulas for excitonic spectra and the manifestation of FEs in linear absorption and in Circular Dichroism spectra.

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