THz charge oscillations and charge transfer in DNA

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We investigate [1, 2] charge transfer in DNA dimers, trimers and polymers (monomer is one base-pair) with a tight binding approach at the base-pair level, using the relevant on-site energies of the base-pairs and the hopping parameters between successive base-pairs [3]. A system of N coupled differential equations is solved numerically with the eigenvalue method, allowing the temporal and spatial evolution of electrons or holes along a N base-pair DNA segment to be determined [1, 2]. We predict electron or hole oscillations in DNA dimers [1, 2] with frequency in the range $f \approx$ 0.25–100 THz (period $T \approx$ 10–4000 fs) i.e. mainly in the mid- and far-infrared with wavelengths $\lambda \approx$ 3–1200 μm [2]. The efficiency of charge transfer between the two monomers which constitute the dimer is described with the maximum transfer percentage p and the pure maximum transfer rate pf. For dimers made of identical monomers $p = 1$, but for dimers made of different monomers $p < 1$. For trimers made of identical monomers the carrier oscillates periodically with $f \approx$ 0.5–33 THz ($T \approx$ 30–2000 fs) [2]; for 0 times crosswise purines $p = 1$, for 1 or 2 times crosswise purines $p < 1$. For trimers made of different monomers the carrier movement may be non-periodic [1, 2]. Generally, increasing the number of monomers above three, the system becomes more complex and periodicity is lost; even for the simplest tetramer the carrier movement is not periodic. The inverse decay length β used for the exponential fit of the pure mean carrier transfer rate $k = k_0 \exp(-\beta d)$, where d is the carrier transfer distance and the exponent η used for the power law fit $k = k_{0'} N^{-\eta}$ are computed [1]. For polymers β falls in the range $\approx 0.2 - 2$ Å^{-1}, k_0 is usually 10^{-2}–10^{-1} PHz although, generally, it falls in the wider range 10^{-4}–10 PHz. η falls in the range $\approx 1.7 - 17$, $k_{0'}$ is usually $\approx 10^{-2}$–10^{-1} PHz, although generally, it falls in the wider range $\approx 10^{-4} - 10^{3}$ PHz. The results are compared with theoretical and experimental works of other colleagues. This method allows assess the extent at which a specific DNA segment can serve as an efficient medium for charge transfer.

References

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