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LECTURE

"Carrier Oscillations within B-DNA Monomers, Dimers, Trimers and Polymers"

Ass. Prof. C. Simserides

Section of Solid State Physics, Department of Physics,

National and Kapodistrian University of Athens

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Carrier Oscillations within B-DNA Monomers, Dimers, Trimers and Polymers

C. Simserides

National and Kapodistrian University of Athens, Department of Physics,
Section of Solid State Physics, Panepistimiopolis, GR-15784 Zografos, Athens, Greece

Abstract

We study, analytically and numerically, electron and hole oscillations within B-DNA monomers (one base pair), dimers (two base pairs) and trimers (three base pairs). We employ two Tight Binding (TB) approaches: (I) at the base-pair level i.e. a wire model and (II) at the single-base level, i.e. an extended ladder model (since it also includes diagonal hoppings) as well as (III) Real-Time Time-Dependent Density Functional Theory (RT-TDDFT). In (I), the site is a monomer i.e. a base pair, while, in (II), the site is a base. The frequency content of the oscillations is in the THz regime. The amplitude of the oscillations is negligible within monomers, but it is 1 for dimers made of identical monomers and homotrimers and less than 1 in other cases of dimers and trimers, according to (I) and (II). We also compare our results from all these three methods [1, 2, 3, 4] in terms of frequency content, maximum transfer percentage i.e. amplitude of oscillations and mean probabilities to find the carrier at the sites and we find that they are in good agreement. The three different methods give complementary aspects of the THz oscillations.

Continuing our work on B-DNA oligomers and polymers [1, 2, 3, 5, 6] we present our new results, on the frequency content of an extra carrier oscillation along periodic, quasi-periodic and fractal B-DNA polymers made of *N* monomers. We employ the two variants of the Tight-Binding approach, (I) and (II), mentioned above. Initially, we focus on the Fourier Spectra of the probabilities to find the extra carrier at each monomer, having placed it at time zero at a specific monomer. The frequency content is in the THz domain. We define the weighted mean frequency (WMF) for each site, a measure of its frequency content. The large-*N* limits of the WMFs, are constants in the THz domain. To obtain a measure of the overall frequency content of carrier oscillations in the polymer, we define the total weighted mean frequency (TWMF), averaging the WMFs of all sites with weight the probability of finding the extra carrier at each site. The large-*N* limit of the TWMF is also a constant in the THz domain.

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