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Thesis Title	*Charge transfer in periodic DNA segments: Tight-Binding description at the base-pair level and at the single base level*
Supervisor	C. Simserides, Assistant Professor
Summary	We employ two Tight-Binding approaches in order to describe single carrier (hole or electron) transfer in some periodic B-DNA segments made up of N base pairs: (I) at the base-pair level, using the on-site energies of the base pairs and the hopping integrals between successive base pairs and (II) at the single-base level, using the on-site energies of the bases and the hopping integrals between neighboring bases, specifically between (a) two successive bases in the same strand, (b) complementary bases that constitute a base pair, and (c) diagonally located bases of successive base pairs. These Tight-Binding parameters are taken from the literature and are used to solve a system of MD coupled equations [$MD = N$ (I), $MD = 2N$ (II)] for the time-independent problem, and a system of MD coupled 1^{st} order differential equations for the time-dependent problem. We solve those systems for three types of periodic B-DNA segments, which are defined by the way the base-pair sequence is constructed. For each of these categories, we study the HOMO/LUMO eigenvalue spectra (eigenspectra), as well as the HOMO/LUMO densities of states (DOS). Then, we calculate the mean (over time) probabilities to find the extra carrier at each site [base pair (I) or base (II)] of a given segment, the Fourier spectra, which reflect the frequency content of carrier transfer, and the pure mean transfer rates $k_{i',i}$ from a certain site to another. The results and conclusions of both our approaches are discussed for the three types of periodic polymers that are studied. Comparison of the two approaches leads to the understanding of complementary aspects of charge transfer through DNA.
Key words	DNA, charge transfer in biological systems, polymers, tight-binding model
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