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| Name-Surname | Marilena Mantela |
| Thesis Title | <i>Charge transfer in aperiodic B-DNA sequences: Tight-Binding description at the base-pair level</i> |
| Supervisor | C. Simserides, Assistant Professor |
| Summary | <p>The subject of this M.Sc. Thesis is charge transfer in aperiodic B-DNA polymeric segments. In the first part, we set the theoretical background of the Tight-Binding Model in order to describe charge transfer at the base-pair level. We examine the behaviour of an extra single carrier (electron or hole) after its placement in a particular monomer (base pair) and study its transfer along the polymer using characteristics such as the on-site energies of the carrier at each base pair and the carrier hopping parameters between the nearest neighboring base pairs. In the second part, we analyse and discuss some features that came of from the application of the Tight-Binding Model in quasiperiodic (Fibonacci, Thue-Morse, Double-Period, Rudin-Shapiro) and fractal (Cantor Dust, Asymmetric Cantor Set) monomer sequences. These features include the HOMO and LUMO eignespectra, the Density of States (DOS), the mean over time probabilities to find the extra carrier in a particular monomer, the frequency content (Fourier spectra) of the transfer of this additional carrier and the pure mean transfer rate of the carrier.</p> <p>Finally, we apply the above analysis to calculate the pure mean transfer rates of some sequences that have been studied in experimental works and we compare our results with the corresponding experimental values.</p> |
| Key words | DNA, charge transfer, aperiodic sequences, tight-binding model |
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