Electronic transport in DNA

The question on whether DNA can conduct electricity, and if so how this can be utilized, has been a subject of discussion particularly since direct experimental results became available. Part of the motivation for such studies is the potential use of DNA in nanotechnology and also the possibility of DNA damage-repair mechanisms via electron transfer. Despite the enhanced activity in both experimental and theoretical studies, the complexity of DNA is still preventing us from forming a consistent understanding.

The project will consist of three levels of refinement:

Calculations of model systems: Of particular interest to us is a 1D model which includes the backbone structure of DNA explicitly and exhibits a semiconducting gap. This model can also exhibit a crossover from an insulating to a nearly conducting state above a certain threshold backbone disorder. The model Hamiltonian is readily investigated using standard techniques from the theory of disordered systems such as, e.g., the transfer-matrix technique (TMM) or the recursive Green function method (GFM) [2]. These techniques allow to study, e.g., the localization lengths of an electron on short DNA strands but also complete chromosomes with many billion of base pairs. Finite temperature can be incorporated via a phenomenological phase breaking length.

Calculations of electronic structure via DFT: In order to further validate the model parameters, we intend to make DFT calculations [3]. We use the Turbomole program to calculate the probability of electron transfer using all-electron DFT calculations. The DFT investigations will build from a small model system (two base pairs) to a large system in which at least one full turn of the helix (ten base pairs) will be explicitly treated.

Correlating transport and biological function: Once a clear picture of the localization and transport properties of DNA has been obtained, it is natural to ask whether these correlate with the biological function of the DNA or related bio-molecules.

The project requires the use of high-performance computational methods such as energy-level statistics and the transfer-matrix method together with finite-size-scaling approaches.

For further information, see http://www.warwick.ac.uk/go/DisQS.

References:
2. for work on the electronic properties of disordered systems, including the methods to be used in the first part of the project, refer to reference [80] of the supervisor.