Electric Properties of the DNA Nucleotides

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In recent years, there has been significant demand and research activity for the development of new DNA sequencing technologies. The achievement in completing the first reference human genome sequence is just the beginning of a revolution that could potentially lead to a genome-based medical practice. For genome-based medical treatment to become a reality, and for medical practitioners to routinely analyze an individual’s DNA in a clinical setting, technology is needed that can perform sequencing cheap and at a speed thousands of times faster than that of the current technology. A technique was proposed [1] based on measurement of transversal conductive properties of a DNA molecule passing between two nanoelectrodes.

Charge transport through biological molecules ultimately depends on the electronic and chemical structure of these molecules, altered by the presence of the nanoelectrodes. Therefore, characterization of the electrical properties of the DNA bases (adenine, cytosine, guanine, and thymine) is a crucial step in developing a DNA sequencing technology. We present a first-principles study of the current-voltage characteristics of the DNA nucleotides (a DNA base with phosphorus-sugar group added), placed in a nanogap between nanoelectrodes, supplying electric bias [2,3]. The quantum transport calculations yields the tunneling regime which strongly vary with the junction and molecule geometry. Results are very sensitive to details of the DFT functionals. We provide understanding of the calculated conductance characteristics, based on analysis of the system molecular levels as well as on the inter-geometrical conformations of the system components.

References:

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