Reading DNA codes

Employing Quantum Tunneling Current in 2D Nano-Structures for Designing Solid-State DNA Sequencing Devices

***A. Kiakojouri, I. Frank**, Institute of Physical Chemistry and Electrochemistry, Leibniz Universität Hannover*

In Short

- Design of a high throughput DNA sequencing device
- Based on Graphene/Boron Nitride 2-D heterostructure materials
- Employing tunneling current for DNA detection
- Based on first-principle calculation ...

DNA is a fundamental part of all living cells. DNA strands contain all necessary information required for growth, function, and heredity of living organisms. Therefore, accessing this information is crucial for life-science researchers. Traditional methods of DNA sequencing are based on complex and expensive chemical procedures, which are time-consuming and have limitations in the length of the DNA strand that can be sequenced. In order to overcome the drawbacks of traditional sequencing methods and to perform DNA sequencing with high speed and low cost, various novel methods were proposed. Among those, the electrical detection of nucleotides with the application of 2-D nanostructures is quite promising. One of the major nano-material candidates for this application is the monolayer form of carbon, known as graphene. graphene's unique electrical and physical characteristic and also, very low thickness makes it a great candidate for the electrical DNA sequencing applications. In this project, the possibility of employing a hybrid 2D nanomaterial based on a Graphene/h-BN lateral heterojunction as a solid-state DNA sequencing device will be investigated. To this end, a novel graphene/h-BN (nanopore)/graphene 2D nanodevice is introduced. Figure 1 illustrates the scheme of graphene and graphene/h-BN nanopore. DNA nucleotides will pass through the nanopore, which is created in the h-BN layer, and modulate the electrical current that flows through the device surface. Due to the insulating characteristic of the h-BN layer, the major charge transport mechanism is shown to have a quantum tunneling nature. The nucleotides of the DNA strand have exclusive molecular characteristics. So, in the presence of each nucleobase within the nanopore, the amount of tunneling current would be different. So, it can be used as a signal to distinguish between different nucleobases. In the present work, we plan to theoretically investigate the translocation dynamics of single-strand DNA through the nanopore, the interaction between device and nucleobases, and the amount of current modulation due to each nucleobase. Figure 2 depicts the placement of nucleotides in nanopore for studying the interaction. We will use the first-principles level of theory, employing Car-Parrinello molecular dynamics (CPMD) for the accurate calculation of dynamical processess at the atomic level and a combination of density functional theory (DFT) and none-equilibrium Greens function (NEGF) formalism, for the calculation of electronic structures and electronic transport.

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https://www.theochem.uni-hannover.de

More Information

Funding

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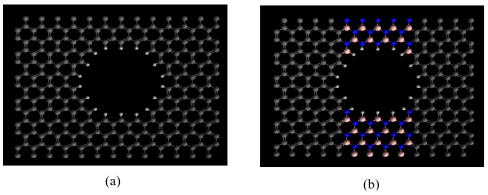

***Figure 1:** (a) Graphene nanopore (b) Graphene/h-BN nanopore.*

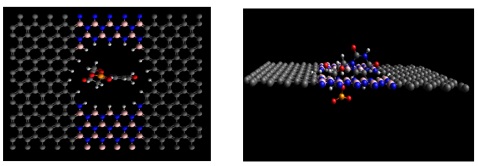

***Figure 2:** Nucleotide placement in G/h-BN nanodevice.*