Reading DNA codes

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

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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, containing all necessary information required for the 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 [1]. 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 [2]. One of the most promising candidates for this application is the monolayer form of carbon, known as graphene. The unique properties of graphene, along with very low thickness makes it a great candidate for the electrical detection approaches [3]. Alongside the advantages of graphene for DNA sequencing application, some challenges persist that need to be addressed [4]. It has been shown that the combination of graphene with similar 2D materials in a lateral heterostructure can substantially improve the device efficiency [5]. 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/hBN (nanopore)/graphene 2D nanodevice is introduced. Figure 1 illustrates the scheme of graphene and graphene/h-BN nanopores. 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

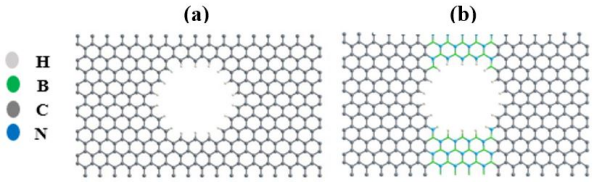

***Figure 1:** (a) Graphene nanopore (b) Graphene/h-BN nanopore.*

have a quantum tunneling nature. The nucleotides of the DNA strand have exclusive molecular characteristics. So, the presence of each nucleobase within the nanopore will cause a distinctive current in the channel, which can be exploited for nucleotide detection. We will use the first-principles level of theory, employing Car-Parrinello molecular dynamics (CPMD) for the accurate calculation of dynamical interactions at the atomic level. Also, a combination of density functional theory (DFT) and non-equilibrium Greens function (NEGF) formalism will be utilized for the calculation of electronic structures and electronic transport. The first phase of the project consisted in studying the nucleotide/device dynamic interaction. To do so, nucleotides are separately placed in the middle of the nanopore, without any initial speed or water molecules, and the interaction of each nucleotide with the nanopore within the G-5BN device (graphene/h-BN/graphene 2D heterostructure with 5 atomic layers of h-BN and a nanopore in the middle of the device) was studied and compared to a pure graphene nanopore. Figure 2 depicts the geometry of nucleotides in the G/5BN nanopore at steady states. Also, the translocation of nucleotides through the nanopore is simulated by applying initial kinetic energy. Commencing with an initial velocity is an essential step for comprehending the orientation and speed variation of the nucleotides as well as the resistance of the nanopore to their passage. Designing an appropriate aqueous system is an important step for studying the nucleotide's behavior in the solvent environment. To do so, we prepared simulation boxes, which are similar in size to the device supercell dimension but different in height, and filled them with water. The nucleotide/device system was merged with the water box, and the additional water molecules were omitted for maintaining the density of the system at around 1 g/cm3. The simulation results indicate that water molecules have their natural Brownian motion and may expand in the simulation box. Also, the influence of water molecules on the nucleotide movement and their interaction

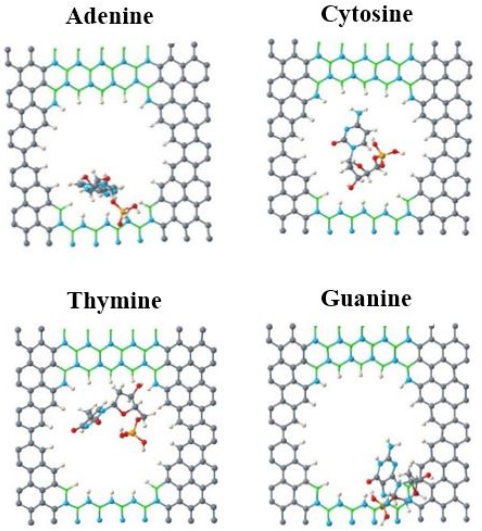

Figure 2: *Geometry of nucleotides in the G/5BN nanopore at steady states*

with nanopore edges is tangible. Figure 3 depicts the interaction of adenine with G5BN nanopore in aqueous and saline solutions. The TranSIESTA soft-

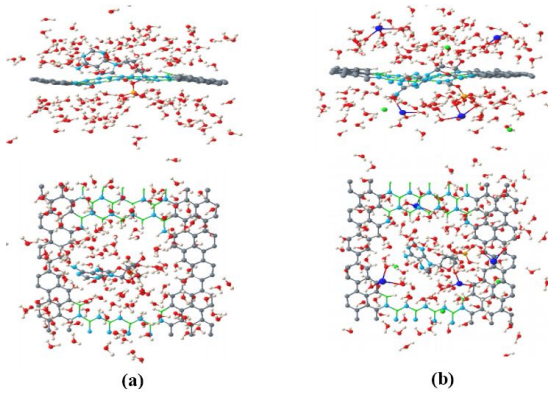

Figure 3: *(a) dAMP interaction with G-5BN nanopore without any charges. (b) dAMP interaction with G-5BN nanopore with ionic charges*

ware package, which is based on NEGF formalism, is adopted for calculating the amount of lateral current and the sensitivity of the G/h-BN nanopore to the presence of nucleotides at different voltages. In this phase, the placement of the nucleotide in the nanopore was relaxed with the DFT geometry optimizer. These simulations have been performed for the G/h-BN nanopore with five and seven BN layers (G-5BN and G-7BN), as well as pristine graphene nanopore as a reference. Figure 4 depicts the sensitivity of devices to the presence of nucleotides, which has been achieved by calculating the lateral current at Vds = 0.5 V. The result indicates higher sensitivity of G/h-BN nanopores to the presence of nucleotide, in comparison to pristine graphene. Progressing of the project leads us into interesting and important

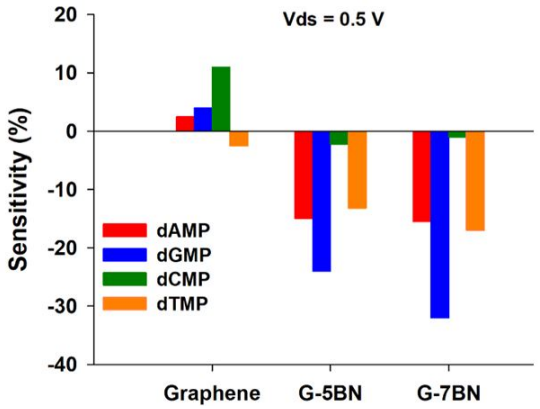

Figure 4: *Sensitivity of graphene, G-5BN and G-7BN devices toward different nucleotides.*

new effects, which are necessary to be further investigated. We have encountered several factors that can influence the sequencing results. We plan to extend the calculations of device-nucleotide interaction to the G-7BN device, which shows promising results in sensitivity calculations. Moreover, the high resistance of water molecules against nucleotide motion is a challenging matter for pushing the nucleotide with initial kinetic energy. So, implementing a practical model for pushing nucleotides through the nanopore in the solvent environment is an important point that needs to be pursued. We will also consider the influence of multi-nucleotides ssDNA on the interaction of each nucleotide with a nanopore and consequently, on the sensitivity of the device. Applying these improvements to the device and system can mitigate the encountered challenges and lead to better optimized devices.

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More Information

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