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 . . .

Figure 1: *graphene and graphene/h-BN/graphene nanopores with 5 and 7 layares of h-BN.*

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
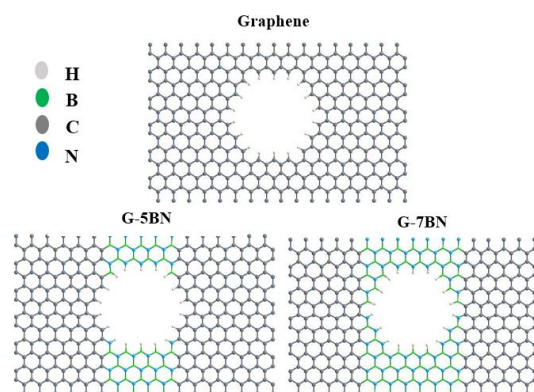
is shown to have a quantum tunneling nature. The nucleotides of the DNA strand have exclusive molecular characteristics. So, the presence of each nucleobase within the nanopore will cause a distinctive current in the channel, which can be exploited for nucleotide detection. We will use the first-principles 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 of 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 within the G-5BN and G-7BN nanopores was studied and compared to a pure graphene nanopore.

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 with nanopore edges is, with and without ionic charges is tangible. Figure 2 depicts the inter-

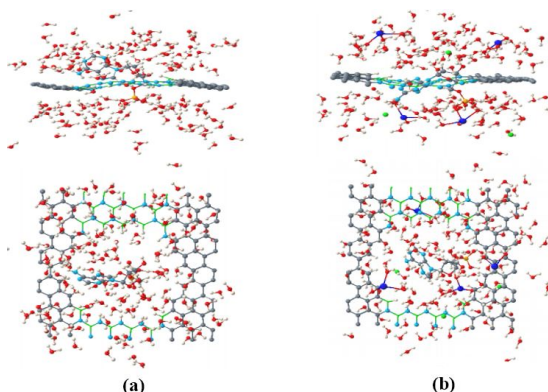action of adenine with G5BN nanopore in aqueous and saline solutions.

Figure 3: *Sensitivity of graphene, G-5BN and G-7BN nanopores towards different nucleotides. (a) Vds=0.5V and (b) Vds=1V.*

Figure 2: *(a) dAMP interaction with G-5BN nanopore without any charges. (b) dAMP interaction with G-5BN nanopore with ionic charges*

The TranSIESTA software 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. The results indicates that the current modulation in nanopores caused by the presence of nucleotides can be divided into two different mechanisms. The first one is the structural deformation in nanopore edges, which is almost the same for all nucleotides and can be attributed to the interaction of a phosphate backbone. The second effect is the electrostatic interaction between the electronegative ends of the nucleotides and the nanopore edges, which is different due to the unique alignment of these ends in each nucleotides [6]. The sensitivity of pristine graphene, G-5BN, and G-7BN nanopore to the presence of nucleotides, at different bias voltages is shown in Fig. 3. It can be concluded that G/h-BN/G heterostructures improve the sensitivity compared to the pure graphene nanopore. Thus, they can provide a promising platform for reliable detection of different nucleotides.

In the next step, the influence of adjacent nucleotides in DNA strands on the interaction with nanopore structures will be considered. To do so, a DNA strand consisting of ten nucleotides in the chain is designed in a manner that resembles a real-world sequencing scenario while maintaining the feasible length for an ab-initio molecular dynamic simulation scenario. the new design is based on a B-form DNA strand with a rotation of 10 bases per turn (BPT),
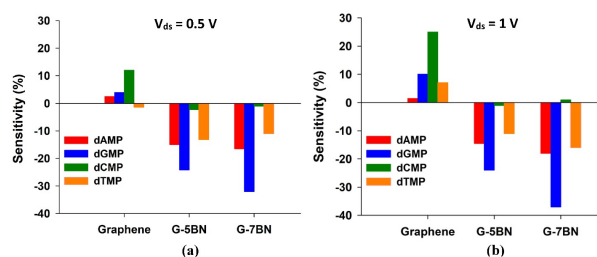
which is the most common form and BPT in the human body. Fig. 4 shows the DNA strand placed in the modified G-7BN nanopore. This model is capa-

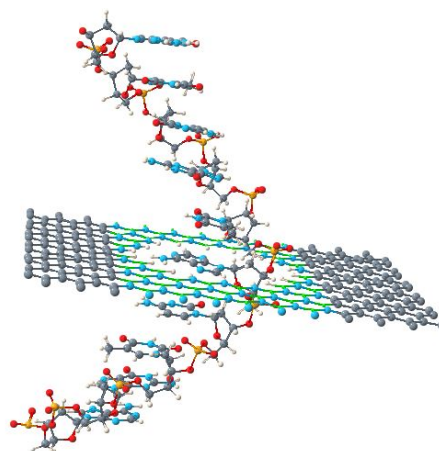
Figure 4: *DNA strand placement in G-7BN nanopore.*

ble of giving the most comprehensive view by taking three important variables into account, namely the interaction of the nucleotides within a DNA single strand, the impact of adjacent nucleotides on nanopore edges, and including the backbones negative charge in the simulation.

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More Information

[1] L. Steinbock and A. Radenovic, Nanotechnology, **26**, 074003 (2015).

[2] B. Venkatesan and R. Bashir, Nature Nanotechnology, **6**, 615-624(2011).

[3] S. Heerema and C. Dekker, Nature Nanotechnology, **11**, 127-136 (2016).

[4] H. Bayley, Nature, **467**, 164-165 (2010).

[5] Q. Li, M. Liu, Y. Zhang and Z. Liu, Small, **12**, 1-1 (2016).

[6] A. Kia, I. Frank and E. Nadimi, PCCP, **23**, 25126-25135(2021).