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Gate-Modulated Graphene Quantum Point Contact Device for DNA Sensing

Anuj Girdhar, Chaitanya Sathe, Klaus Schulten, and Jean-Pierre Leburton

Abstract

In this paper, we present a computational model to describe the electrical response of a constricted graphene nanoribbon (GNR) to biomolecules translocating through a nanopore. For this purpose, we use a self-consistent 3D Poisson equation solver coupled with an accurate three-orbital tight-binding model to assess the ability for a gate electrode to modulate both the carrier concentration as well as the conductance in the GNR. We also investigate the role of electrolytic screening on the sensitivity of the conductance to external charges and find that the gate electrode can either suppress or enhance the screening of biomolecular charges in the nanopore depending on the value of its potential. Translocating a double-stranded DNA molecule along the pore axis imparted a large change in the conductance at particular gate voltages, suggesting that such a device can be used to sense translocating biomolecules and can be actively tuned to maximize its sensitivity.

Keywords

QPC; Nanopore; Simulation; Device

1 Introduction

The past few years have experienced a surge in the search for low-cost, next-generation biomolecule sensing technologies [1, 2]. Recent advances in the fabrication of solid-state nanopores (SSNs) offer promising alternatives to conventional DNA sensing methods [3–8]. In this context, the use of graphene as the membrane of a SSN device is advantageous, because its sub-nanometer thickness can scan a molecule passing through the nanopore with a resolution comparable to the DNA nucleotide spacing [9]. Recently, the implementation of graphene nanopores for molecular detection has been demonstrated experimentally [10–13], whereas molecular dynamics studies have suggested the possibility of sequencing of DNA by ionic current blockades through these nanopores [14, 15]. Additionally, first-principles-based calculations have advocated identifying DNA nucleotides in SSNs by measuring their influence on the electronic current across graphene layers [16–19].

Graphene nanoribbons (GNRs) are narrow strips of graphene with electronic states that are strongly dependent on edge boundary conditions imparted on the electronic wave functions [20–23]. Owing to the particular shape of the GNR edge, the boundary conditions can

become quite complex. The presence of a nanopore itself acting as a scatterer introduces additional boundary conditions which, in turn, can profoundly affect the electronic states of GNRs [24–26].

In a previous work, we performed a thorough investigation of the effects of geometry and carrier concentration (via the Fermi energy) on the conductance sensitivity of a patterned GNR [16]. It was shown that the response of the conductance is significantly enhanced by modulating the Fermi energy in constricted quantum point contact (QPC) geometries. We chose a QPC geometry because the unique boundary conditions of the edge make the nanoribbon conductance particularly sensitive to changes in external potential energy (see ref. [16] for a more in-depth discussion of the effects of geometry on nanoribbon conductance sensitivity). However, in that work the Fermi energy, which determines the local of the GNR's local electrostatic environment due to the presence of charges in the system from other materials making the membrane. In this paper, we consider a multilayer graphene membrane operating as a field-effect transistor (FET) for which a back-gate electrode in the membrane controls the carrier concentration in the graphene layer. By adjusting the voltage of the back-gate, we determine the resulting electrostatic potential in the GNR, which modulates the carrier concentration $n(\mathbf{r}) = n(\mathbf{r}, V_G)$ and thus the conductance sensitivity.

To assess the viability of this multilayer device to enhance the conductance sensitivity of a QPC GNR, we show that different gate electrode biases can significantly alter the electron concentration of the GNR. In addition, different gate biases also enhance the GNR conductance response to positional changes of a DNA molecule passing along the nanopore axis. Finally, we analyze the effect of hydrogen passivation by using tight-binding models involving an expanded basis set and compare our results with a single-orbital basis approach without Hydrogen passivation.

2 Background and Methods

2.1 Multilayer Device Description

A schematic diagram of the proposed multilayer device is shown in Fig 1. The device consists of a single-layer, 59 Carbon site (7.13 nm) wide armchair graphene nanoribbon with Hydrogen passivation of any dangling bond in a QPC geometry between two SiO₂ layers to insulate the GNR from the solution and the back-gated electrode. The layer thickness of the top (bottom) oxide layer is 10 nm (65 nm). Underneath the bottom oxide is a 2 nm thick metal gate electrode, which will be used to vary the carrier concentration as explained below. A double-conical nanopore resulting from ultra-bright electron lithography processing [27], with the smallest diameter of 2.4 nm at the same location as the graphene layer, is present through the center of the entire stack.

When an oxide comes into contact with an aqueous salt solution, a chemical reaction between its surface atoms and the solution creates a static layer of charge on the oxide surface [28, 29]. We take this into account by including a small 1 nm-thick layer of charge $\sigma = 10^{12} \text{ cm}^{-2}$ in units of e , the electronic charge. Because the magnitude of the charge is

strongly dependent on particular choice of oxide, salt, and solution pH, we treat σ as an adjustable parameter which can be optimized for the particular device application.

2.2 Self-Consistent Determination of Electric Potential

In order to calculate the electronic transport properties of the graphene nanoribbon, we first obtain the electrostatic potential on the GNR due to external charges in the membrane device. To this end, we self-consistently solve the Poisson equation for a 3D box containing the multilayer device immersed in solution with a Newton-multigrid method to obtain the electric potential $\phi(\mathbf{r})$ [16].

$$\nabla \cdot [\epsilon(\mathbf{r}) \nabla \phi(\mathbf{r})] = -e \left[K^+(\mathbf{r}) - Cl^-(\mathbf{r}) \right] - \rho_{\text{fixed}}(\mathbf{r}). \quad (1)$$

Here, ϵ is the local permittivity. The right-hand-side charge term includes ions in solution (K^+, Cl^-) and fixed charges ρ_{fixed} such as dielectric surface charge and/or DNA charge present in the SSN. We assume the electrolyte distributions obey Boltzmann statistics [4]

$$K^+(\mathbf{r}) = c_0 \exp \left[-\frac{e\phi(\mathbf{r})}{k_B T} \right], Cl^-(\mathbf{r}) = c_0 \exp \left[\frac{e\phi(\mathbf{r})}{k_B T} \right] \quad (2)$$

Here, K^+ and Cl^- are the local ion concentrations, e is the electronic charge, and c_0 is the molar concentration of KCl. We assume that the base concentration is 100 mM. In addition, we assume that a typical translocation bias across the membrane is less than 0.5 V, a regime in which eq. 2 is valid [30]. The system is discretized onto a nonuniform $129 \times 129 \times 129$ point grid, with a higher grid resolution around the graphene nanopore region. Neumann boundary conditions are imposed on the sides of the box, while the top of the box is subject to a Dirichlet boundary condition $V_{TOP} = 0$. The gate electrode layer also is subjected to Dirichlet conditions, and is held at V_G , which we vary.

Once eq. 1 is solved, the resulting potential in the nanopore graphene layer can be used to calculate its carrier concentration and transport properties.

2.3 Electronic Transport Properties of Graphene Nanoribbons

For this purpose we use a formalism based on the tight-binding approximation, in which the Hamiltonian for a graphene nanoribbon can be written as [20,31]

$$H = \sum_{i,\mu} [\epsilon_\mu - e\phi(\mathbf{r}_i)] a_i^{\mu\dagger} a_i^\mu + \sum_{\substack{\langle i,j \rangle \\ \mu\nu}} V_{\mu\nu}(\mathbf{n}) a_i^{\mu\dagger} b_j^\nu + V_{\nu\mu}(\mathbf{n}) b_j^{\nu\dagger} a_i^\mu \quad (3)$$

where ϵ_μ is the on-site occupation energy of an electron in state μ located at site i , e is the magnitude of the electronic charge, $\phi(\mathbf{r}_i)$ is the electric potential at site i obtained from eq. 1, and $a_i^{\mu\dagger}/b_i^{\mu\dagger}$ and a_i^μ/b_i^μ create and annihilate electrons in state μ at site i for the graphene A/B sublattice, respectively. The states μ, ν are the p_z , d_{yz} , and d_{zx} orbitals of monatomic Carbon as opposed to solely including the p_z orbital in traditional tight-binding models of graphene [32]. This expanded basis improves the accuracy of the electronic structure as well as

allowing for the inclusion of edge-passivation by Hydrogen. The values of the transfer integrals $V(\mathbf{n})$ are determined by fitting these parameters to *ab initio* calculations and depend on $\mathbf{n}$, the unit displacement between sites i and j [32]. The values for all on-site energies and transfer integrals are taken from ref. [31].

Once the Hamiltonian is determined, the electronic properties of the graphene nanoribbon can be calculated by using the Non-Equilibrium Green's Functions (NEGF) technique. The Green's function $\mathbf{G}$ is given in the operator representation as

$$\mathbf{G}(E) = [E - \mathbf{H}]^{-1} \quad (4)$$

or in real space

$$[E \pm i\eta - H(\mathbf{r}, \mathbf{r}')] G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (5)$$

where $\mathbf{H}$ is the Hamiltonian of the system and η is infinitesimally small. If we discretize the real space coordinates to correspond to positions on the lattice, we can divide the device into three sections, two leads (L) on either side of a conductor (C).

$$\begin{bmatrix} G_L & G_{LC} & 0 \\ G_{CL} & G_C & G_{LC} \\ 0 & G_{CL} & G_L \end{bmatrix} = \begin{bmatrix} E - H_L & V_{LC} & 0 \\ V_{CL} & E - H_C & V_{LC} \\ 0 & V_{CL} & E - H_L \end{bmatrix}^{-1} \quad (6)$$

If $V_{LC} = V_{CL}^\dagger$, eq. 6 yields

$$G_C = \left[(E + i\eta) I - H_C - \sum_{\alpha} \Sigma_{\alpha} \right]^{-1} \quad (7)$$

where $\Sigma_{\alpha} \equiv V_{\alpha C}^\dagger [E - H_{\alpha}]^{-1} V_{\alpha C}$ is the self energy of lead α . For modelling different conductors with identical leads, $[E - H]^{-1}$ only needs to be calculated once.

The transmission function, which is used to find the conductance, can be determined from the Green's function. The transmission $T(E)$ between the leads 1 and 2 is given by [33]

$$\bar{T}_{12} = -Tr \left[(\Sigma_1 - \Sigma_1^\dagger) G_C (\Sigma_2 - \Sigma_2^\dagger) G_C^\dagger \right]. \quad (8)$$

The conductance across the conductor at a particular bias V_{DS} can be expressed as

$$G = \frac{2e}{V_{DS} h} \int_{-\infty}^{\infty} \bar{T}(E) [f_1(E) - f_2(E)] dE \quad (9)$$

where $f_{\alpha}(E) = f(E - \mu_{\alpha})$ is the probability an electron occupies a state at energy E in the lead α , $\mu_1 - \mu_2 = V_{DS}$ is the bias across the conductor. μ_1 is taken to be the Fermi energy of the conductor, calculated by enforcing charge neutrality in the graphene layer. In all subsequent

calculations it is assumed that $f(E)$ is the Fermi-Dirac distribution function and the temperature is 300 K.

Along with the transmission function, the local density of states (LDOS) can be determined from the Green's function.

$$\rho(\mathbf{r}, E) = -\frac{1}{\pi} \text{Im} [G(\mathbf{r}, \mathbf{r}, E)] \quad (10)$$

This can then be used to find the local electron (hole) concentrations in the conduction (valence) bands.

$$n_e(\mathbf{r}) = 2 \int_{E_c}^{\infty} \rho(\mathbf{r}, E) f(E - e\phi(\mathbf{r})) dE \quad (11)$$

$$n_h(\mathbf{r}) = 2 \int_{-\infty}^{E_v} \rho(\mathbf{r}, E) (1 - f(E - e\phi(\mathbf{r}))) dE \quad (12)$$

where $e\phi(\mathbf{r})$ is the local electrostatic potential energy, and E_c (E_v) is the bottom (top) of the conduction (valence) band. When calculating the local electron concentration, the LDOS is assumed to be that of an isolated GNR.

A flowchart describing an overview of the computational steps required to obtain the electrical response of a graphene transistor to the motion of biomolecules is shown in figure 2. Each computation step, outlined in blue, generates the input for the next computation step.

3 Results

3.1 Gate-Modulated Carrier Concentration

We first investigate the carrier concentration response due to changing the bias of an external gate electrode in the multilayer structure described above. The bottom gate bias was set to values between $V_G = -4$ V to 4 V in 1 V intervals. For each gate bias value, the potential of the entire system was calculated from eq. 1, and inserted into the Hamiltonian. It is assumed that the source and drain leads are held at 0 V.

Figure 3 a (above) shows the local electrical potential in the graphene layer at $V_G = -4$ V, 0 V, and 4 V. Due to the negative charge layers present on the oxide surfaces in contact with water, the potential in the GNR is less than zero at a $V_G = 0$ V, especially away from the pore. The potential in and around the immediate vicinity of the nanopore remains unchanged by gate bias changes as a result of heavy screening by the electrolytic solution, thereby maintaining a potential value of approximately 0 V inside the nanopore for all gate biases. The effects of screening decrease significantly further inside the GNR, away from the pore. Near the GNR leads ($|x| = 7.5$ nm), the potential increases by over 200 mV as the gate voltage is increased from $V_G = -4$ V to 4 V. This potential change corresponds to a Fermi energy variation of approximately .2 eV, consistent with the magnitude of the Fermi energy parameter changes in our previous work[16]. This implies that a gate electrode in this configuration can significantly alter the carrier concentration. The electric potential at these three gate biases along the x axis at $y = 0$ is shown in the lower portion of Fig. 3 a.

Figure 3 b shows the electron (left) and hole (right) concentrations in a QPC GNR in the multilayer device as a function of gate potential. For $V_G = -4$ V, far from the nanopore, in the GNR, the large negative local potential (-150 mV) pushes the effective Fermi level far below the conduction band, reducing the electron concentration to negligible levels. For the same reason, the hole concentration is largest at this gate voltage, exceeding $5 \times 10^{12} \text{ cm}^{-2}$ at some locations. Because of ion screening, the effective potential in the GNR near the pore remains slightly below zero at all gate voltages is changed. This produces a very small but nonzero electron concentration around the nanopore edge, which varies negligibly as the gate voltage is changed. Similarly, the hole concentration around the pore varies slightly as the gate voltage is increased and is quite large compared to the electron concentration due to the effect of the oxide surface charge, exceeding $4 \times 10^{12} \text{ cm}^{-2}$ for $V_G = -4$ V at various locations around the pore. Owing to the boundary conditions imparted by the nonuniform QPC edge as well as by the nanopore, the local density of states varies around the nanopore. As a result, there is a similar variation of the local carrier concentrations around the perimeter of the pore. The QPC in this study has x- and y- axis reflection symmetry about the nanopore center, and as a result, the carrier concentration also acquires these reflection symmetries[16].

At larger gate biases, the electron concentration away from the pore is significantly increased, achieving values of over $2 \times 10^{12} \text{ cm}^{-2}$ at $V_G = 4$ V. The hole concentration responds in the opposite way, becoming negligible far from the nanopore at the largest gate voltage, though remaining significant in the vicinity around the nanopore. These large variations in carrier concentration arising from gate voltage modulation demonstrate the tunability of the conductance properties of the graphene transistor. The spatial distribution of the electrons depends on the particular geometry used, and can be tailored to the specific application by changing the edge geometry appropriately. The linear carrier density at these three gate biases along the x axis, averaged over the y axis, is shown in the lower portion Fig. 3 b.

At all gate biases, the hole concentration is significantly larger than the electron concentration due to the large negative potential arising from the oxide surface charge. In addition, there is an inherent asymmetry between the conduction and valence bands due to the three-orbital basis used in our model[31]. Both of these are consistent with the location of conductance minimum at non-zero gate biases in experimental systems[34].

A vertical cross section of the absolute electric potential of the entire system at $V_G = -4$ V is displayed in Figure 4 a. Because of ion screening, the potential is approximately zero almost everywhere in solution. However, in the center of the nanopore in the graphene plane, the potential is negative due to the close proximity of the oxide surface charge. This is indicative of the screening length of the ions which allows the potential originating from a charge in the pore to penetrate significantly into the nanoribbon. On the sides of the multilayer stack, the potential gradually increases from a value of -4 V at the gate electrode to -50 mV at the top of the upper oxide layer. The double-conical shape of the nanopore allows the potential of the stack resulting from the gate electrode to be focused onto a majority of the graphene layer. The specific geometry of the pore and stack can be adjusted

to enhance or weaken the influence of the gate electrode on the graphene potential and thus carrier concentration.

The electrolyte distribution in the center of the nanopore at $y = 0$ at various gate biases is shown in Figure 4 b. For $V_G = -4$ V, the K^+ concentration reaches a value over 120 mM in the pore center. Close to the pore wall, the negative surface charge causes an accumulation of K^+ ions in excess of 140 mM. The situation is opposite for Cl^- ions, reaching concentrations of 85 mM and 70 mM in the pore center and wall, respectively.

As the potential is increased, the K^+ and Cl^- concentrations decrease and increase respectively, as the potential in the center of the nanopore increases. K^+ ion concentration in the center of the pore decreases by almost 20 mM, and decreases by 30 mM near the pore wall. For Cl^- ions, the concentration in the pore center increases by 10 mM, while at the pore wall it increases by 15 mM. The larger changes in concentration at the pore wall are a result of diminished screening at those locations.

There is a vertical asymmetry of the potential in the pore due to the position of the gate electrode, also appearing in the electrolyte distribution. This is most evident for $V_G = 4$ V, where the Cl^- concentration is clearly larger in the lower half of the nanopore. The geometry of the pore could be modified to enhance this asymmetry, especially through the use of an additional gated layer near the graphene plane. This can be used to alter the ionic conductance properties of the nanopore [35].

3.2 Conductance Modulation from dsDNA Translocation

We calculated the electric potential in the graphene layer due to the presence of a 10 base pair poly-AT double-stranded DNA (dsDNA) molecule in different vertical positions within the nanopore. For each gate voltage, the potential was calculated with and without a DNA strand in the pore. For the former situation, the DNA center of mass was held at three different positions on the nanopore (z) axis : in the plane of the graphene layer, 1.25 nm below the graphene plane, and 2.5 nm below the graphene plane. The center of mass of the DNA was maintained the same x and y positions, namely on the axis of the pore. The conductance was calculated assuming that the leads are biased such that they are charge-neutral, offsetting the influence of the charged oxide substrate.

As seen in the upper portion of Fig. 5 a, the conductance of the GNR without a DNA strand is enhanced for positive and negative gate voltages, because the former and latter create additional electrons and holes, respectively. However, the conductance is larger for positive gate voltages due to the presence of the oxide surface charge in addition to the inherent asymmetry between the valence and conduction bands of the QPC.

Because there is a low concentration of carriers near the pore, the conductance is relatively small, ranging from 1 to 3 μS over the gate voltage range. The presence of a DNA molecule in the nanopore significantly enhances the conductance for all gate voltages, because of the emergence of carriers near the pore as a result of electric potential of the DNA charges. For positive gate voltages, the multilayer stack acquires a net positive potential, and the K^+ concentration is significantly reduced near the pore wall. As a result, the screening of the

negative charges on the DNA is mitigated, and the DNA has a stronger effect on the local carrier concentration and thus the conductance. At negative voltages, there is a larger accumulation of K^+ ions around the pore wall, reducing the impact of the local gating due to the DNA charge.

As the DNA is translated along the z axis, the potential in the plane of the graphene sheet due to the DNA charges appears as if the DNA is rotating. As a result, the local carrier concentration around the nanopore as well as the conductance are both altered due to the different DNA positions. As seen in Fig. 5 a (above), the change in DNA position translates to a conductance difference of nearly $6 \mu S$ at $V_G = 2$ V which is nearly six times the conductance difference at $V_G = -4$ V. Changing the gate potential can significantly alter the sensitivity of the conductance to the positional changes of external charges in the nanopore. The asymmetry in the conductance about the gate voltage can be attributed to the presence of the surface charges on the oxide layers.

In order to compare the expanded basis of our tight-binding model with the traditional, single p_z orbital tight-binding model of graphene, we performed the same calculation with the simpler basis. As seen in the lower portion of Fig. 5 a the conductance resulting from the expanded basis is over one order of magnitude larger than that from the traditional model. In addition, in the simpler model the gate voltage associated with the minimum conductivity for all DNA positions was found to be 2 V, whereas at this gate voltage the use of the expanded basis model results in a very large conductance.

The large differences between these two models can be attributed to two factors, namely Hydrogen passivation allowed by the expanded basis model as well as the more complex boundary conditions introduced by the additional terms in the expanded Hamiltonian. Figure 5 b shows the transmission functions for the GNR using the expanded basis with H-passivation, the expanded basis without H-passivation, and the single-orbital basis without H-passivation. The effective gap for the GNR with the expanded basis with passivation is much smaller than those gaps without passivation. This is due to the fact that the Hydrogen atoms make the effective GNR width slightly larger. In addition, the Fermi energy is closer to the conduction band in this basis. As a result, all conductances are higher in the case of passivation with the expanded basis. An interesting feature in all three cases is the existence of additional states within the gap, arising from the constricted QPC edge. These manifest themselves as transmission resonances, occurring at very narrow energy ranges, whose exact position depends on the particular basis used.

The three-orbital basis corrects many deficiencies of the single-orbital model, namely the inability to reproduce the presence of band-gaps in all GNRs, the asymmetry between valence and conduction bands, and the ability to incorporate Hydrogen-passivation[31]. Further additions to this basis would serve to add minor corrections to the overall electronic structure and would not change the global properties of the system.

It should be noted that though the expanded basis set imparts significant changes to the electronic structure around the band gap, the fundamental behavior of our device remains unchanged. Because of the complex boundary conditions of the edge and nanopore,

conduction channels can open or close within very narrow energy ranges, allowing minor Fermi energy changes, via a gate electrode or external charges, to cause significant variation in the device conductance regardless of the particular basis used. This is the underlying principle behind our device.

4 Conclusion

In this paper, we present a comprehensive model that describes the electronic properties of a gated multilayer device containing a graphene nanoribbon as a bio-sensing layer. We show that the use of a multilayer membrane device for biomolecule sensing offers great advantages because of its ability to actively control the electronic properties of the graphene sensing layer, thereby enhancing its sensitivity to passing in the pore.

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Fig. 1.

(a) A diagram of a graphene transistor with a single-layer graphene (SLG) nanoribbon sandwiched between two oxide layers. (b) (above) Top view of the QPC GNR with nanopore. (below) Cross-sectional schematic diagram of the simulated multilayer device, displaying all parameters chosen for the simulation. These figures are not to scale.

Fig. 2.

Overview of the computational model used to calculate the electronic properties of graphene nanoribbons in a multilayer transistor device. Computational steps are boxed in blue, yielding results that are used as input for the next computational step.

Fig. 3.

(a) (above) Color plots of the local electric potential in the graphene layer at three gate voltages (-4V, 0V, 4V). (below) Potential profile through the center of the nanopore within the graphene plane at three gate voltages. (b) (above) Local electron (left) and hole (right) concentration in the QPC at the same gate voltages. (below) Total carrier concentration profile along the current propagation direction, averaged along the width (y axis) of the nanoribbon.

Fig. 4.

(a) Vertical cross section of the absolute electric potential of the system through the nanopore center at $V_G = -4$ V. (b) Spatial distribution of electrolytic ions in solution at various gate voltages.

Fig. 5.

a) (above) GNR conductance versus gate bias for different DNA positions along the nanopore axis using the expanded three-orbital basis. (below) GNR conductance versus gate bias using the traditional single-orbital tight-binding model of graphene. b) The electron transmission versus energy around the Fermi energy for the expanded three-orbital basis (solid black), the expanded basis without Hydrogen passivation (dashed green), and the single orbital basis without Hydrogen passivation (dashed red).