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To cite this article: Asma Wasfi *et al* 2020 *New J. Phys.* **22** 063004

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Deutsche Physikalische Gesellschaft DPG
IOP Institute of Physics

Published in partnership with: Deutsche Physikalische Gesellschaft and the Institute of Physics

OPEN ACCESS

RECEIVED
18 December 2019

REVISED
23 March 2020

ACCEPTED FOR PUBLICATION
8 April 2020

PUBLISHED
12 June 2020

PAPER

DNA sequencing via Z-shaped graphene nano ribbon field effect transistor decorated with nanoparticles using first-principle transport simulations

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Keywords: graphene nano ribbon, nano pore, field effect transistor, nanoparticle, first principle, DNA sequencing

Abstract

DNA detection has revolutionized medical and biological research fields. It provides a wealth of medical information for each individual, which can be used in a personalized medicinal procedure in the future. Genome sequence helps to enhance our perception of inheritance, disease, and individuality. This work aims to improve DNA sequencing accuracy and the overall current signal using a novel nano pore based sensor that is developed to detect and identify the DNA bases. Herein, a novel z-shaped field effect transistor with a nano pore for the aim of DNA detection is studied, where a gate terminal is added below the center of the z-shaped graphene nano ribbon. First-principle transport calculations are used to identify the DNA bases and electronic signature. An efficient density functional theory approach combined with non-equilibrium Green's function formalism (DFT + NEGF) are utilized to detect the transmission spectrum and current for DNA nucleo bases: Adenine, Thymine, Guanine, and Cytosine. Using transmission current, a distinctive electronic signature is generated for each DNA base to detect each DNA sequence. Various orientations and lateral position for each DNA base are considered. Moreover, the effect of decorating the developed DNA sensor with gold and silver nanoparticles on the sensor's electrical current and transmission spectra is studied and analyzed. The results suggest that the z-shaped sensor could achieve DNA sequencing with high accuracy. The practical implementation of this work represents the capability to anticipate and cure diseases from the genetic makeup perspective.

1. Introduction

DNA sequencing plays a critical role in genetic risk identification and personalized medicine process. Genome sequencing research field is growing due to the need for faster and cheaper sequencing technologies. Nano pore based sensors are of the most competitive sequencing approaches since they are label free, amplification free, and provide high throughput DNA detection [1, 2]. Nano pores are categorized into three groups: biological, artificial, and hybrid nano pores. Biological pores are usually placed within lipid bilayers, liposomes, and polymer membranes [3]. The first biological nano pore sensor was fabricated with α-hemolysin protein within a lipid bilayer [4].The main types of biological nano pores are α-hemolysin [5], mycobacterium smegmatis porin A (MspA) [6], and Phi29 [7]. Biological pores can be used in DNA sequencing due to their flexibility, sensitivity, and simplicity [3]. However, many problems are facing biological nano pore based sensors such as size restrictions and limited stability [3]. Biological pores limitations push researchers to research alternative solutions such as solid state nano pores [8, 9]. A major advantage of solid state pores is the flexibility to produce them in different shapes and sizes [9]. Furthermore, solid state pores can be developed with different materials such as SiC, SiO_2, and Al_2O_3 [2, 8, 10]. High stability is a main merit of solid-state pores over biological pores [3]. Hybrid nano pores combine

the best features of biological and solid state pores. The hybrid pores idea was initially proposed by Hal *et al* who placed α-HL proteins in SiN film [11]. The main concept of DNA sequencing via nano pore is that when a DNA strand translocates across the nano pore, its ionic current is affected by each nucleo base differently. Therefore, the ionic current crossing the nano pore can be utilized to determine the sequence of DNA bases.

Material choice to fabricate nano pore based devices for DNA detection has critical considerations. Among several materials, graphene has drawn much interest in the development of DNA sequencing devices due to its unique characteristics and structures. Graphene is a material that has unique characteristics which offers novel opportunities for genome sequencing. Due to graphene's exceptional and unique electrical and structural characteristics, it has a great possibility to be used in electronic field effect transistors (FETs) [12]. Graphene is considered a perfect material for nano pore based DNA sequencing since a graphene membrane thickness is 0.35 nm which is almost comparable to the interval among DNA bases [13]. Decorating graphene membrane with metal nanoparticles affects the membrane sensitivity and selectivity [14]. Various nanoparticles (NPs) such as gold (Au) are commonly used to enhance its performance due to their recognized easy functionalization chemistry [15].

Graphene nano ribbons (GNR) are graphene sheets cut in specific patterns. The two types of GNRs, based on their edges, are armchair graphene nano ribbon (AGNR) and zigzag graphene nano ribbon (ZGNR) [16]. ZGNR is metallic while AGNR is either semiconducting or metallic [17]. Metallic AGNR has a width of $\mathrm{Na} = 3p + 2$ where p is a positive integer, while semiconducting AGNR has a width of $\mathrm{Na} = 3p + 1$ or $\mathrm{Na} = 3p$ [17].

Various theoretical and experimental researches were conducted to enhance DNA detection approaches using graphene nano pores. Solid state nano pore based sensors have three sensing strategies based on tunneling, field effect, and ionic current [18]. Among different biological and solid-state nano pores utilized for DNA sequencing, graphene nano pores offer great potential to achieve successful DNA sequencing due to graphene's single atom thickness [19]. Both field effect sensing and ionic current techniques have been successfully performed using graphene nano pore based sensors [20, 21]. In the ionic current technique, a negatively charged DNA strand passes across a nano pore where a bias voltage is applied. The ion flow blockage can be detected where each base has a unique effect. A DNA base is detected by the time it takes to go through the pore and the average blockade magnitude [22]. Graphene is being excessively utilized in field effect transistor construction because of its high mobility of both electrons and holes and unique band structure [23]. Its conductance gives response to DNA base translocations [24]. Theoretical studies showed that each base interaction with graphene result in a unique electrostatic potential signature [25]. Moreover, graphene high conductance allows higher current than ionic current [24, 26, 27]. Thus, graphene field effect transistors are expected to provide faster sequencing speed and higher signal to noise ratio [24].

Since the minimum feature size of electronic sensors is aimed to be reduced to reach atomic scale, it is critical to study the effects on sensing properties of a single atom in device simulations. Various electron transport simulations are developed based on non-equilibrium Green's function (NEGF) formalism [28, 29]. The system electronic structure can be calculated by *ab initio* approach using first principle such as density functional theory [30–33], or using semi-empirical approaches such as extended Hückel (EH) [34] or Slater–Koster tight-binding [35]. In this work, first principle approach is used since it provides high predictive power and gives more accurate results without prior experimental data. The charge transport of the present sensor is investigated when different DNA bases are placed within the nano pore using Quantum-ATK software. The sensor device is produced using atomistic structure of a z-shaped field effect transistor with a nano pore. Then, the device geometry optimization by Quantum-ATK first principle transport simulation is achieved where the density functional theory is utilized. Next, the sensor electronic properties such as transmission spectrum and current are generated by employing density functional theory with non-equilibrium Green's function. The results reveal that each base has a distinctive signature because of the different chemical and electronic structure of each base. The electrical signatures of DNA bases change with their orientation and translation. The aim of this study is to improve the sensor sensitivity by adding a gate terminal to the z-shaped graphene nano ribbon introduced in previous work [36]. Furthermore, the effect of graphene decoration with silver and gold nanoparticles and interaction between graphene and the nanoparticles on electronic structure are examined.

2. Sensor setup and configuration

2.1. Setup of the z-shaped field effect transistor with a nano pore

The structure of the nano-scale sensor is developed and investigated using Quantum-ATK simulator as shown in figure 1. The sensor field effect transistor is made of graphene channel. Graphene nano ribbon is

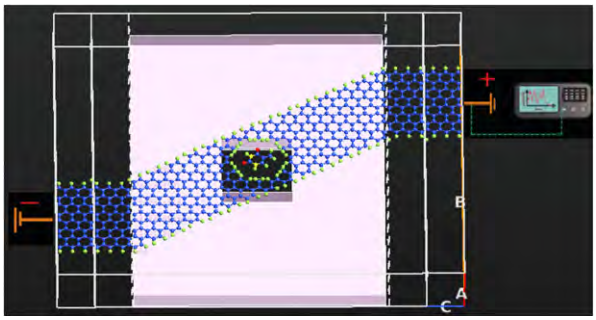

Figure 1. Schematic diagram of the z-shaped graphene nano ribbon field effect transistor with a pore. DNA nucleo bases pass through the nano pore and transverse electronic current pass across the graphene membrane. The gate potential (2V) and bias voltage between the right and left electrodes (+0.25 and −0.25 eV) are fixed. The nano ribbon and nano pore edges are passivated by hydrogen. Color-code: carbon-blue, nitrogen-yellow, oxygen-red, and hydrogen-green.

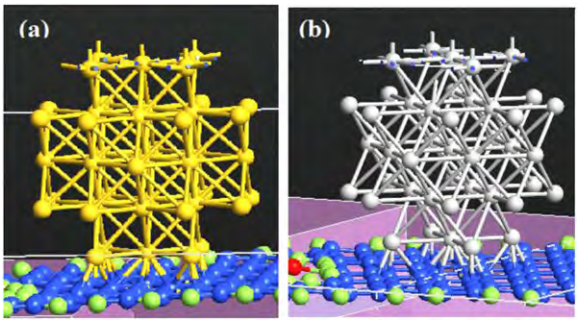

Figure 2. (a) Optimized 10 Å gold (111) nanoparticle. (b) Optimized 10 Å silver (111) nanoparticle.

made of source and drain and a semiconducting channel. The sensor is a three terminal device with source, drain, and gate. The gate potential enables the calculation of transmission spectrum and current. A nano pore of size 10.1 Å is placed in the middle of the z-shaped nano ribbon. The field effect transistor is made of two metallic zigzag graphene nano ribbon electrodes connected through a semiconducting channel of armchair graphene nano ribbon. The metallic zigzag nano ribbons have sixteen carbon chains in width each, and the semiconducting armchair has thirteen chains in width (length of the metallic ZGNR electrodes is 15 Å while the width of the armchair graphene nano ribbon is 16.61 Å). Two layers: dielectric (with a dielectric constant 4) and a metallic are added under the central armchair graphene nano ribbon. No doping for the source, drain, and gate is performed. The edge carbon atoms of the nano ribbon and nano pore saturated their dangling bonds by bonding with their neighbor atoms. The edge carbon atoms are passivated with hydrogen. This type of transistor is called a z-shaped graphene nano ribbon transistor [37]. The field effect transistor is investigated for the aim of DNA sequencing using density functional theory combined with non-equilibrium Green's formalism (DFT + NEGF). The DNA backbone contribution is neglected since the backbone noise can be identified and deducted from the DNA bases signal [38].

2.2. Configuration of the sensor decorated with nanoparticles

Decorating graphene with metal nanoparticles influences graphene charge transport behavior since the nanoparticles change graphene local electronic structure. Metal nanoparticles such as silver (figure 2(b)) and gold (figure 2(a)) are selected in this work since they have high affinity to DNA nucleo bases. The z-shaped sensor is decorated with 10 Å gold (figure 3(a)) and silver (figure 3(b)) nanoparticles. The structure of nanoparticles are optimized using quantum-ATK. The nanoparticles' influence on local electronic structure is studied using electronic properties such as transmission spectrum and current. Here, the electronic effect of attaching silver and gold nanoparticles to the z-shaped sensor on the DNA base detection is investigated.

The nanoparticles are generated in our lab inside an ultra-high vacuum (UHV) compatible system by magnetron sputtering and inert-gas condensation techniques [39]. The distribution of the deposited nanoparticles on a substrate is random, thus, random locations are selected in this work.

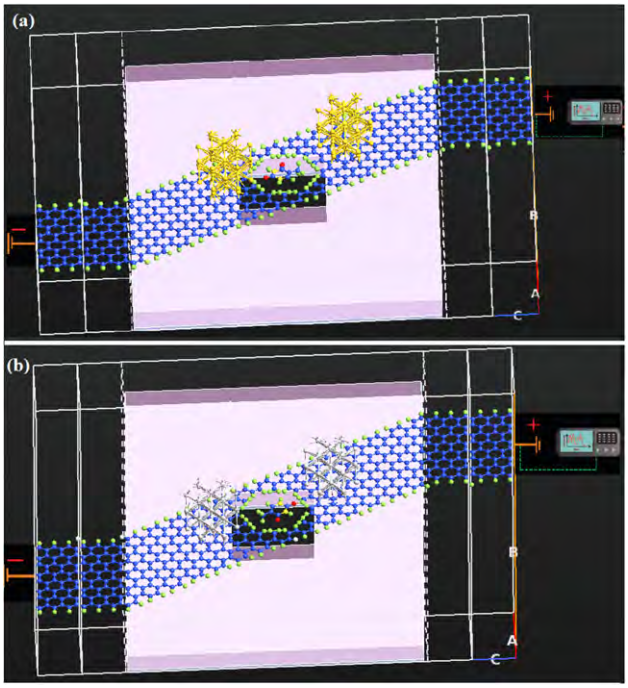

Figure 3. (a) Z-shaped graphene field effect transistor with a nano pore decorated with 10 Å gold nanoparticles. (b) Z-shaped graphene field effect transistor with a nano pore decorated with 10 Å silver nanoparticles.

3. Computational methodology

Prior to studying the electronic properties for the developed sensor, a geometry optimization is performed. All optimizations are exceled by density functional theory as configured in quantum-ATK–DFT package. Generalized gradient approximation (GGA) [40] is used for the exchange and correlation functions. In order to expand the Kohn–Sham (KS) orbitals, 400 eV is used for the cutoff energy for the plane wave basis set. K-points of $1 \times 1 \times 1$ are used within Monkhorst–Pack scheme for the Brillouin zone integration. Structural relaxation is performed for all atoms to ensure that the Hellmann–Feynman forces are less than 0.05 eV/Å.

The electronic transport properties are calculated by NEGF + DFT simulations integrated in the quantum-ATK package. Quantum-ATK–DFT is also used to calculate and simulate the transmission spectrum. Poisson equation with marginal conditions is utilized where Neumann boundary condition is applied to A and B directions which are perpendicular to the transport direction while Dirichlet boundary condition is applied to C direction. The Neumann boundary condition ensures that the electrostatic potential is constant and its derivative is zero. This is a suitable boundary condition when the sensor has a metallic gate.

Perdew–Zungar (PZ) parameterization of the local density approximation (LDA) and Troullier–Martins norm-conserving pseudo potentials are selected for exchange correlation of quantum-ATK–DFT calculator [41]. The pseudo-atomic local orbitals are single zeta polarized at hydrogen and carbon atoms and double zeta polarized at rest. $1 \times 1 \times 50$ k-points are used for the Brillouin zone integration within Monkhorst–Pack scheme. A 75 Hartree mesh cut-off is used to calculate the charge density. A 200 sampling points are used within the range -2 to 2 eV, the gate voltage is set to 2 V, and the applied bias voltage among the right and left electrodes is set to 0.5 V. In this work, the transverse current is measured for the various DNA bases' orientation. The resulting current varies for each DNA base orientation giving a distinctive current interval for each base making it possible to distinguish between the four DNA bases.

The zero bias transmission spectrum among the source and drain electrodes is found as [42, 43]:

$$T(E) = \mathrm{Tr}\left\{\Gamma_D(E)\, G(E)\, \Gamma_S(E)\, G^{\dagger}(E)\right\} \tag{1}$$

where, Tr is the trace, E is the energy, $\Gamma_{D,S}(E) = i\left[\sum_{L,R}(E) - \sum_{S,D}^{\dagger}(E)\right]$ characterizes the broadening level due to the coupling to the electrodes, i indicates iteration, and $\sum_{L,R}(E)$, $\sum_{S,D}^{\dagger}(E)$ are the self-energies displayed by the source and drain.

The bias transmission spectrum is calculated using NEGF formalism, as inserted in quantum-ATK, using [42]:

$$T(E, V_b) = \mathrm{Tr}\left\{\Gamma_D(E, \mathrm{V_D})\, G(E)\, \Gamma_S(E, \mathrm{V_S})\, G^{\dagger}(E)\right\} \tag{2}$$

where, G and $G^{\dagger}$ are correlated with the main scattering region of advanced Green's function, and $V_b = V_s - V_d$ where $V_b$is the bias voltage among source (V_s) and drain (V_d). R, L, D, and S refer to the right, left, drain, and source. The probability for quantum mechanical transmission of electrons is referred by the transmission spectrum function $T(E, V)$. The self-energies $\sum_{L,R}(E)$ and $\sum_{S,D}^{\dagger}(E)$ in the effective Hamiltonian are created to detect the right and left electrodes' semi-infinite effect.

Integrating $T(E, V)$ over the energy window is calculated using the difference of the Fermi functions $f_{S,D}(E) = \{1 + \exp[(E - E_F - eV_{S,D})/k_B T]\}^{-1}$ gives the total current [42]:

$$I = \frac{2e}{h}\int_{-\infty}^{\infty} \mathrm{d}E\, T(E, V)\left[f_S(E) - f_D(E)\right] \tag{3}$$

where, $f_{S,D}$ is the Fermi function of the macroscopic reservoirs into which S and D are the electrodes , I is the total current, e is the electron charge and its value is exactly $1.602\,176\,634 \times 10^{-19}$ C , and h is the Planck constant and its value is $6.626\,070\,15 \times 10^{-34}$ J.s.

4. Results and discussion

In this work, it is noticed that each of the four DNA bases (Adenine, Thymine, Guanine, and Cytosine) within the pore results in a unique change in the sensor transmission spectrum and current.

4.1. Transmission spectrum

Figure 4 shows the z-shaped field effect transistor with a nano pore transmission spectra which are calculated by quantum-ATK-DFT. Figure 4 displays the transmission spectra of the z-shaped sensor that contains a bare nano pore and with gold and silver nanoparticles at 0.5 bias voltage and 2 V gate potential. It is noticed that the low value of transmission spectra within the energy range −1.4 to −0.1 eV correspond to the energy window of the central semiconducting AGNR band gap. The transmission spectra displayed in figure 4 indicate that sensor current without gold or silver nanoparticles is higher than that with gold and silver nanoparticles.

During DNA strand translocation process through the graphene nano pore, various orientations of the nucleo bases are probable within the graphene pore. It is therefore critical to take into account how the base orientations affect the transmission spectra. Calculations of transmission spectra are done by placing each DNA base within the pore with four various angular orientations.

It is noticed that the transmission function has different effect depending on the base types. The DNA nucleo bases are classified into two groups: pyrimidine bases containing Cytosine (C) and Thymine (T), and Purine bases containing Adenine (A) and guanine (G). These two groups are different in sizes where purine bases are bigger than pyrimidine bases which lead to stronger coupling and smaller separation for adenine and guanine. Therefore, figure 8 reveals that purine bases resulted in lower current than pyrimidine bases.

Figure 5 shows the four types of DNA bases corresponding to the orientation 0°, while figure 6 shows the bases rotated from 0° to 180° around the x-axis, xy-plane, and xz-plane. The transmission spectra and current are not affected by how the right and left electrode voltages are applied and only relies on the difference between the electrodes' voltages. The effect of DNA bases translation on the transmission spectrum is studied where each DNA base is translated along the z-axis by ±1 Å. Each base is moved 1 Å to the left direction and 1 Å to the right direction as displayed in figure 7. Figure 8 displays the transmission spectra as a function of energy for the sensor with a nano pore at room temperature (300 K). The various panels display the different bases within the nano pore (A, C, G, and T). Each panel shows the transmission spectra for each base due to the four orientations displayed in figure 6. Each panel shows that the four orientations have similar transmission characteristics resulting in a unique current interval for each base. Moreover, the transmission spectra for the different panels vary in their transmission characteristics and number of transmission peaks. In the transmission spectra calculation, the DNA backbone of phosphate and sugar is ignored since it can be detected and subtracted from the bases transmission spectrum.

The transmission spectra change due to the lateral transition for each base is displayed in figure 9. The figure shows how a transmission spectrum is influenced slightly by the radial translation. This slight change in transmission spectrum resulted in currents within a unique current interval for each base.

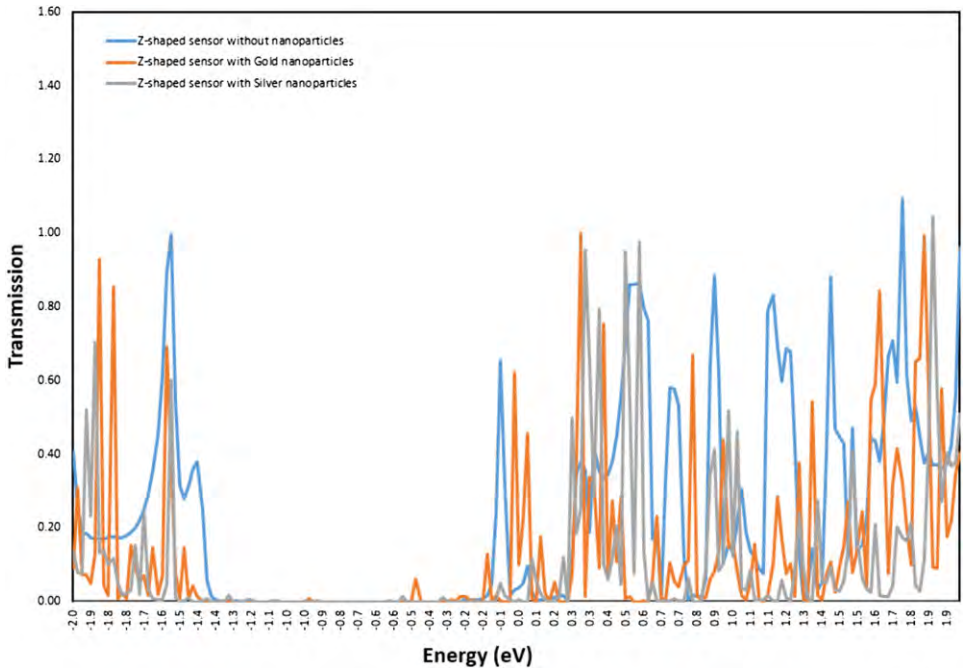

Figure 4. Transmission spectra of the z-shaped graphene field effect transistor with a nano pore (0.5 V bias voltage and 2 V gate potential) for bare sensor as well as for sensors with silver and gold nanoparticles.

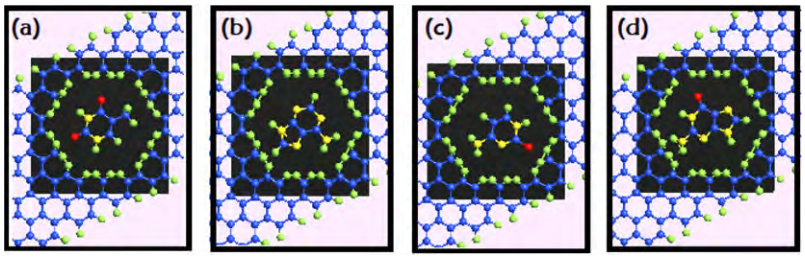

Figure 5. The four DNA bases with a 0° angel: (a) Thymine, (b) Adenine, (c) Cytosine, and (d) Guanine.

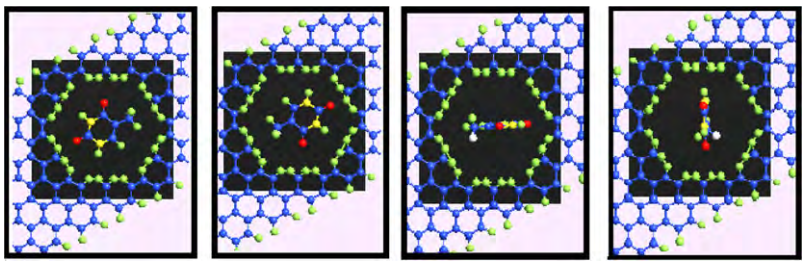

Figure 6. (a) Thymine within the pore at 0° angle. (b) Thymine at 180° angel corresponding to the *x*-plane. (c) Thymine at 180° angel corresponding to the *xy*-plane. (d) Thymine at 180° angel corresponding to the *xz*-plane.

Figure 10 displays the transmission spectra for Cytosine within the nano pore of the z-shaped sensor: bare as well as with silver and gold nanoparticles. The transmission spectra for Cytosine of bare sensor reveal higher and more pronounced current compared with sensor that includes nanoparticles.

4.2. Current

Figure 11 reveals the current for the four angular orientations and the translation for each DNA base within the z-shaped sensor nano pore. To generate an electrical transmission spectrum, a gate potential of 2 V is fixed and the voltage among the right and left electrodes is fixed as +0.25 and −0.25 V. For DNA detection

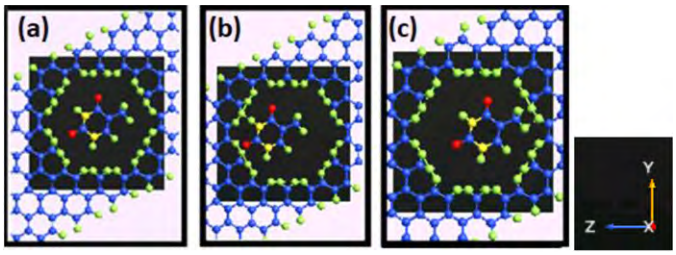

Figure 7. (a) Thymine within the pore at 0° angle. (b) Thymine due to −1 Å translation along the *z*-axis. (c)Thymine due to 1 Å translation along the *z*-axis.

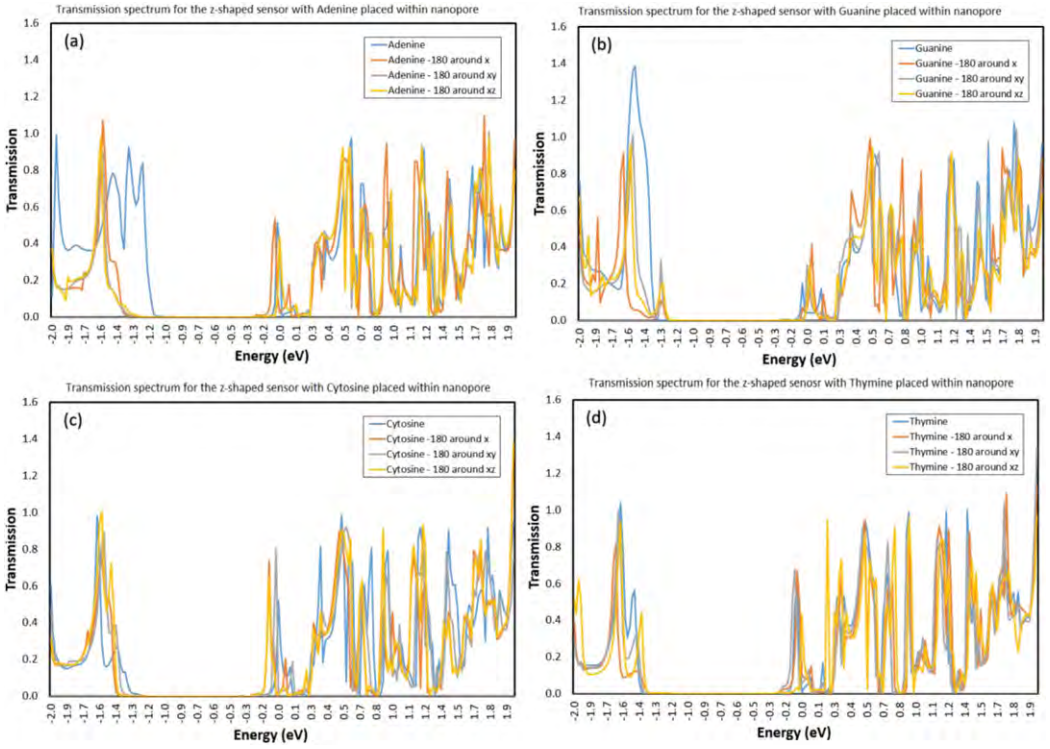

Figure 8. Transmission spectra of the z-shaped graphene field effect transistor with a nano pore at 0.5 V bias voltage and 2 V gate potential for the four types DNA bases: (a) Adenine, (b) Guanine, (c) Cytosine, and (d) Thymine. The transmission spectra colors refer to the base orientation within the sensor nano pore.

via nano pore, the current is the measured value rather than the transmission spectrum. Thus, the transverse current is calculated by integrating the transmission spectra as shown in equation (3). For a specific DNA base orientation displayed in figures 6(a)–7(d) and translation displayed in figures 7(a)–(c), the current variations are displayed in figure 11(a).

Figure 11 displays how each DNA base placed within the sensor nano pore modify the sensor room temperature current. When bases orientations with respect to the nano pore change as in figure 6 and when bases are translated along the *z*-axis, the current change within the ranges displayed in figure 11(b). The DNA current detection is achieved at bias voltage = 0.5 V where the current is of the order of microampere. This current is predicted to be higher than the noise resulting [44] from DNA structure fluctuations while trans locating through the nano pore. Underneath the channel, a gate made of metal is added in order to have a three terminal device which is eventually a FET device. The gate is supplied with 2 V. Figure 11 reveals that the resulting currents are at the microamperes level which indicates much better sensitivity compared to the previous published paper [36].

The phosphate and sugar backbone is adjacent to the nucleo bases which affects the current modulation. However, it is expected that these factors will result in small noise on the resulting current which is systematic and can be deducted. Since this kind of noise is systematic, it can be possibly detected and eliminated as well as the fluid fluctuations while passing through the nano pore [38, 48]. The resulting transverse current for each base is anticipated to be higher than the DNA fluctuations and the effect on the

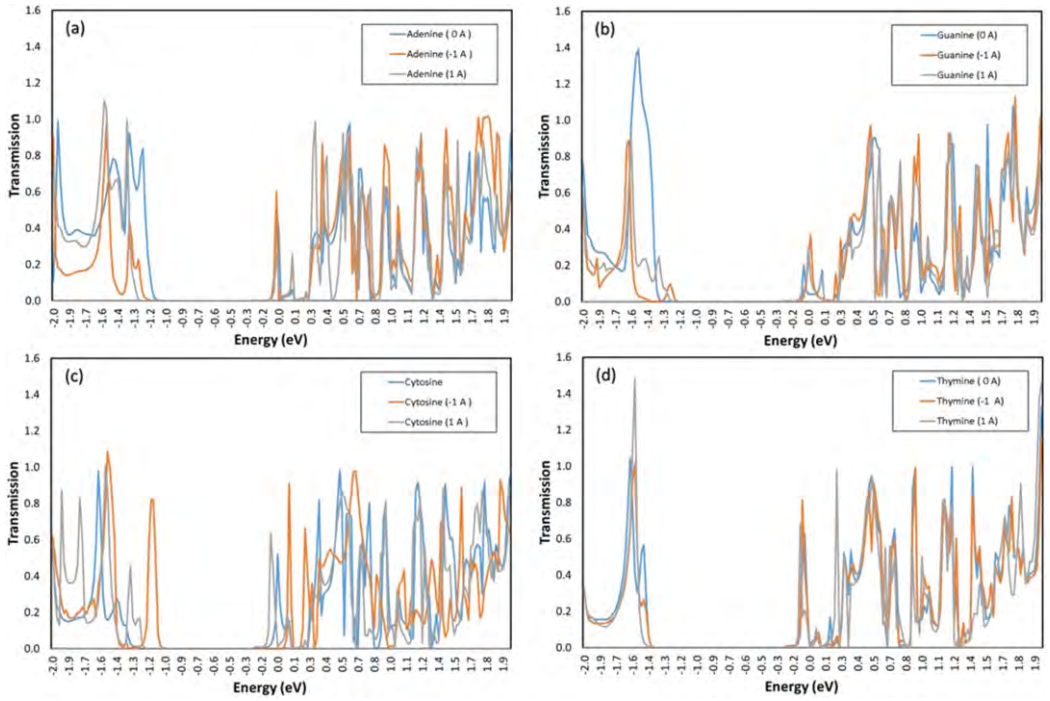

Figure 9. The transmission spectra change due to ±1.0 Å translation along the *z*-axis for: (a) Adenine, (b) Guanine, (c) Cytosine, and (d) Thymine. The transmission spectra colors refer to the base orientation within the sensor nano pore.

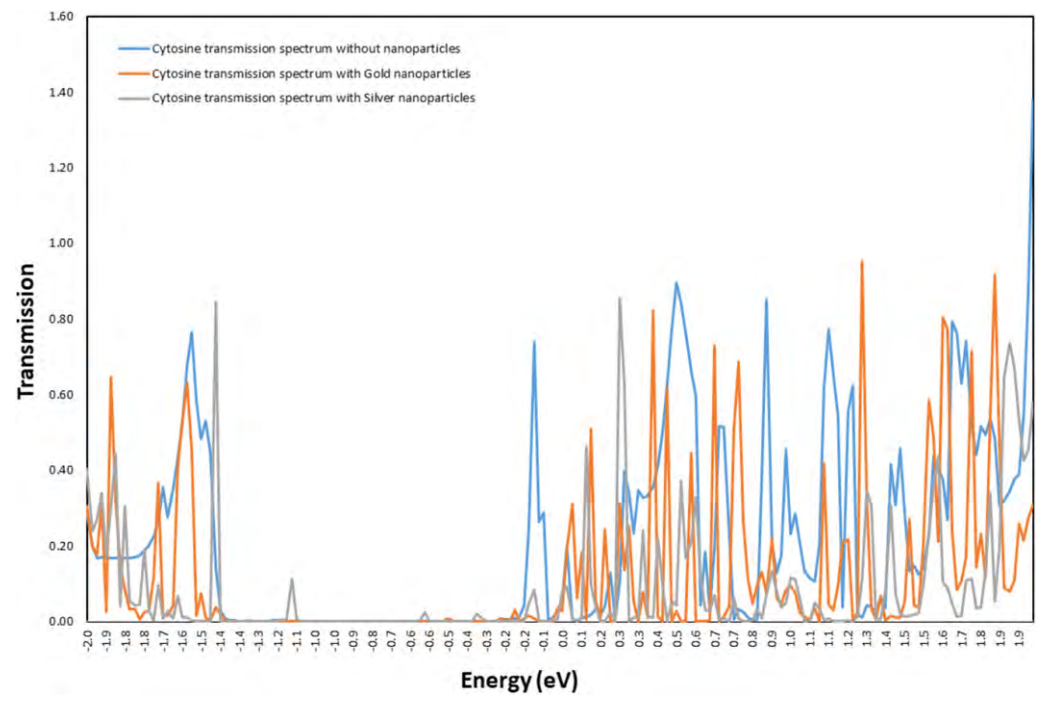

Figure 10. Transmission spectra of the z-shaped graphene field effect transistor with a nano pore for Cytosine at 0.5 V bias voltage and 2 V gate potential for bare sensor as well as with silver and gold nanoparticles.

electronic structure of DNA nucleotides within salt solution [26, 47, 49]. Previous studies show that the noise resulting from sugar-phosphate backbone can be detected and deducted from the general spectra [38, 48]. This kind of simplification refers to the possibility of isolating the signal from the individual bases by subtracting the noise resulting from the sugar-phosphate backbone. The nucleotides current change is expected to be small and within the intervals in figure 11(b).

The nano pore diameter of 1 nm allows one single nucleotide to translocate at a time as displayed in figure 12. The nano pore size of 1 nm is suitable for single stranded DNA sequencing which agrees with

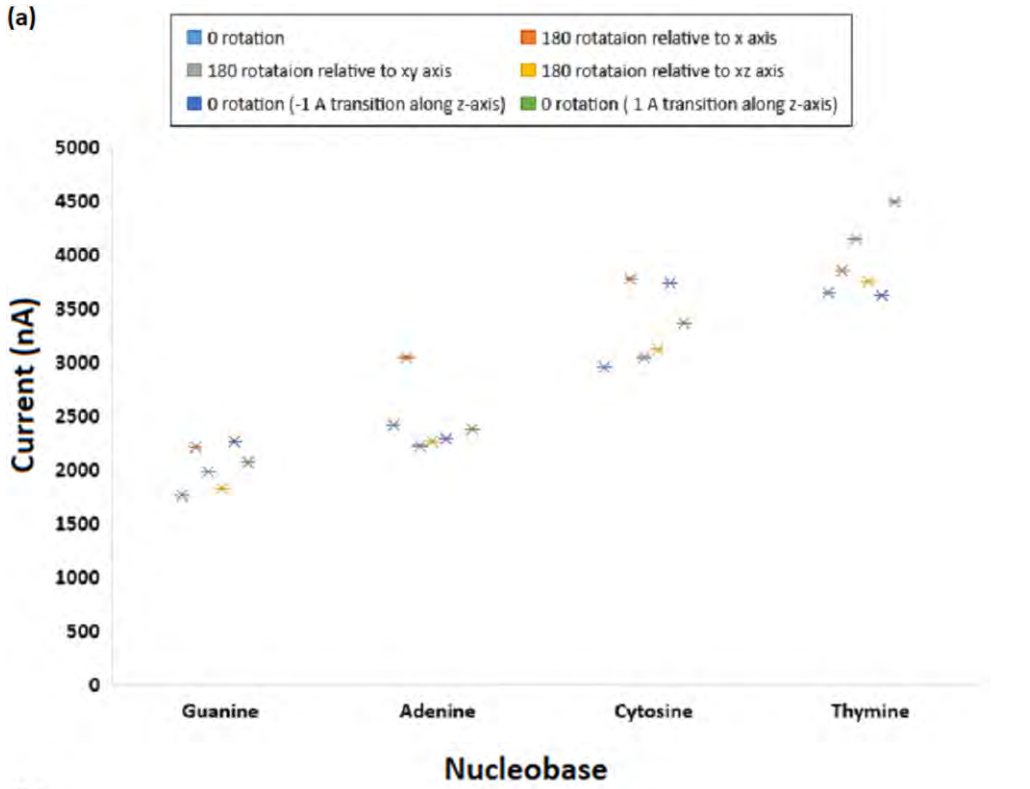

Figure 11. (a) Current difference due to nucleo base various orientations and lateral translation in the z-shaped field effect transistor sensor nano pore. (b) Current ranges due to nucleo base various orientations and translation. Both figures are produced using 0.5 V bias and 2 V gate potential.

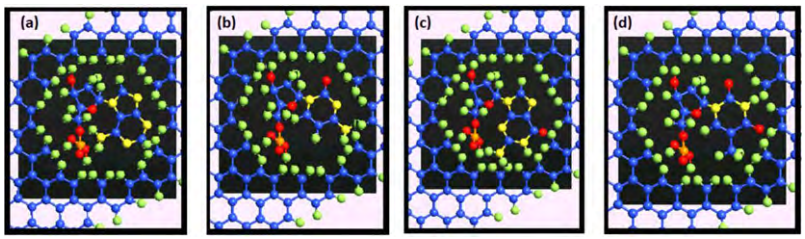

Figure 12. (a) 2′-Deoxyadenosine-5′-monophosphate. (b) 2′-Deoxycytidine-5′-monophosphate. (c) 2′-Deoxyguanosine 5′-monophosphate. (d) 2′-Deoxythymidine-5′- monophosphate.

other studies [45, 46]. The ideal nano pore diameter is 1 to 1.5 nm [26, 47] which allows the single stranded DNA to go through it in unfolded state with a large and readable transverse current.

The real sensor application will include a substrate below the nano ribbon such as SiO_2 or Si_3N_4 underneath. The substrate and solvent effects are not considered in our proof-of-concept simulations and are left for a future work. It should be noted that other studies conducted DNA base detection without considering the substrate and solvent effects [26, 49]. Also, future work may include electronic transport

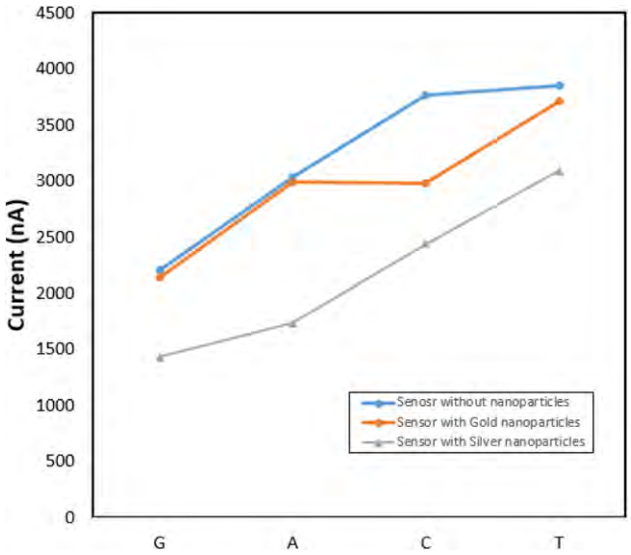

Figure 13. The room-temperature current of the z-shaped sensor when each of the four DNA bases (A, C, G, T) is placed within the nano pore center bare and with gold and silver nanoparticles.

calculations for DNA nucleotides in a salt solution. This work focuses on utilizing z-shaped graphene nano ribbon transistor as a possible sensor for DNA sequencing which showed very good results.

Since the DNA bases are very similar, they can be distinguished by their electronic state, size, and interaction with the nano pore. Each base density of states contribution at the Fermi level is unique due to the different spatial extension of each base. This contribution is highly affected by the bases orientation and geometry. The transverse current is highly sensitive to atomic scale variations, orientation, and distance. That is why specific configurations are preferred for DNA passage through a nano pore.

From the transmission spectrum, it is noticed that the variation of physical and chemical structures between pyrimidine and purine bases affects the coupling between the DNA bases and the sensor that result unique current to make it possible to differentiate the different groups of DNA bases under a specific applied bias voltage. It is also noticed that purine bases including guanine and adenine have lower current than pyrimidine bases thymine and cytosine. Each DNA base has its unique electrical signature that varies slightly due to the various DNA bases orientation. DNA bases affect the nano pore charge density within the surrounding area leading to unique current. The current is multiple orders of magnitude greater than the transverse current utilized in previous sensors [36, 49].

Figure 13 displays the current signature for each DNA base for bare sensor and with gold or silver nanoparticles. The low current in nanoparticle decorated z-shaped sensor is predicted due to various reasons. Firstly, the silver and gold nanoparticles presence can work as a charge scattering sites which reduce the device mobility. Secondly, the nanoparticles placement may lead to poor sp^2 carbon structure recovery. A critical point is that placing metal nanoparticles results in degradation in charge transport properties of graphene sensors [50]. Moreover, it is noticed that DNA bases detection current for the sensor with silver nanoparticles is less than the detection current with gold nanoparticles. The sensor with silver nanoparticles exhibits higher contact resistance than with gold nanoparticles on the applied voltage. The higher resistance of silver nanoparticles is probably due to the space charge field established by the trapped carriers. It is noticed that the sensor mobility with nanoparticles is less than the bare sensor mobility.

5. Comparative analysis

Theoretical studies to enhance the current across nano gaps [47, 51] or nano pores [16, 36, 52] offer moderate improvement. Moreover, applying high bias to obtain high current signal may lead DNA backbone attraction, or breakdown the sensor at high electric field. Unlike other recent sensors based on transverse electronic properties which use small current across a nano pore or a nano gap resulting in low signal, the present device enhances electrical current results from nano ampere to microampere [36] thus makes it easier to detect, measure, and read. Placing a DNA base within the pore affects the charge density resulting in a unique current for each base. The current sensor provides high readable currents when small bias voltage is applied. This may remove the need to reduce the DNA translocation speed since the speed to measure the current may be high which reduces the Brownian fluctuations in blurring the signal. The

present sensors, bare and decorated with nanoparticles, exhibit higher sensitivity in comparison with the previous work [36]. It was found that the bare sensor has the highest sensitivity for DNA bases detection and outperforms the ones decorated with gold and silver nanoparticles. Moreover, the sensor decorated with gold nanoparticles has higher sensitivity than the one decorated with silver nanoparticles. The current difference is due to the variation in the sensors mobility where the bare sensor has the highest mobility, then the sensor with gold nanoparticles, and the least mobility is for the sensor with silver nanoparticles.

Previous studies [53] showed that although the signal of un doped ZGNRs can be influenced by the DNA existence within the pore, it is still hard to differentiate between the different DNA bases. Adding a gate terminal can improve the results by shifting the Fermi energy from the charge neutrality point. Both nano gap and nano pore based sensors lose their efficiency in distinguishing the DNA bases if their size increase [54]. The current z-shaped FET nano pore diameter is 10.1 Å which is effective to identify the different DNA bases. The utilized nano pore diameter is comparable to the nano gap diameter (11 Å) used by Scheicher *et al* [45]. Moreover, the sensor nano pore edge carbon atoms are passivated with hydrogen which reduces the DNA translocation speed and enhance the measurement accuracy for DNA sequencing [45]. Hydrogen prevents the DNA bases from bonding with the graphene membrane and the nano pore. The present observations are in a good agreement with McFarland *et al* [48] and our previous work [36] where the results indicate that the pyrimidine bases within the pore result in higher current than purine bases at 0.5 V bias voltage. Each DNA base has its unique chemical and electronic structure that result in its unique current signature.

It is noticed that decorating the graphene membrane of the developed sensor with gold or silver nanoparticles results in lower current since gold and silver nanoparticles reduce the device mobility. The results of lower current are consistent with previous studies [50, 55, 56]. The DNA bases detection of current for the sensor with silver nanoparticles is less than the detection current with gold nanoparticles since the sensor mobility with silver nanoparticles is lower than its mobility with gold nanoparticles.

6. Conclusion

In conclusion, a novel z-shaped field effect transistor with a nano pore is investigated using first-principle quantum-ATK transport simulations for rapid DNA detection. Transport simulations based on density functional theory combined with non-equilibrium Green's function formalism (DFT + NEGF) are utilized. The DNA detection is achieved by analyzing the electronic transport properties including transmission spectrum and current for the sensor with bases placed within the nano pore. The study illustrates that each DNA nucleo base result in a distinctive modulation of transmission spectrum and current. The sensor has the advantage of large signal of microampere at low bias voltage making it possible to find out the DNA sequence. Moreover, the effect of decorating the sensor with gold and silver nanoparticles, which have high affinity to DNA bases, on sensor signal is studied. It is observed that the bare sensor produced higher electronic current than the sensor decorated with gold and silver nanoparticles. Moreover, the sensor decorated with gold nanoparticles has higher electronic current than the sensor with silver nanoparticles. The mobility of bare sensor is the highest, then the sensor decorated with gold nanoparticles, and finally the one decorated with silver nanoparticles.

Acknowledgments

The authors would like to acknowledge the financial support by United Arab Emirates University (Zayed Center for Health Sciences) with Fund number 31R128.

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