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# DFT-NEGF simulation of graphene-graphdiyne-graphene resonant tunneling transistor

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ABSTRACT

The chemical stability of graphene and graphdiyne means that they can be stacked in different combinations to produce a new nanotransistor for ultra-high frequency applications. Here we report a resonant tunneling transistor through a graphene-graphdiyne-graphene heterojunctions sandwiched between two graphene electrodes. The characteristics of this transistor, which were modeled on the basis of density functional theory, revealed that the current is dominated by tunneling transitions.



## 1. Introduction

According to Moore's law, the number of the components per square inch in the integrated circuits is expected to double every two years. However, continuation of scaling has faced serious limitations and the most important are the fabrication technology and the device performance, as the critical dimension shrinks below 22 nm. These limitations can be overcome by selecting new materials used in the channel of the transistor. Fabricating the devices with extremely small channels may allow making the transistors with small dimensions and higher speeds, without encountering the harmful effects that restrict their performance [1–10].

Carbon nanostructures have great potential to be used in fabricating for high performance transistors. Graphene-based transistors have been developed rapidly and are now considered as an option for post-silicon nanoelectronic devices, due to its distinct electronic properties. In order to control the electron transition in future graphene transistors, graphene needs a non-zero band gap, having semiconducting behavior instead conducting. Researchers have developed methods to significantly opening band gap in graphene such as applying electric field, doping certain atoms, stretching and squeezing [11–18].

Resonant tunneling transistors (RTTs) which were first introduced by Capasso and Kiehl [19] in 1985, have attracted great attentions due to their potential for a wide variety of logic and signal-processing applications. Until now, RTTs made of different materials, have been studied by many researchers [20–25]. Mishchenko et al. have reported the resonance peak and negative differential conductance in combination of a hexagonal boron nitride barrier layer sandwiched between two graphene electrodes. They demonstrated how these heterojunctions induce a tunable radiofrequency oscillatory current so can be used in high-frequency devices [26]. A resonant tunneling high electron mobility transistor based on GaN was designed by Subhra Chowdhury et al., using the ATLAS SILVACO simulator. Their results indicate that GaN based resonant tunneling diode exhibited a peak to valley ratio (PVR) of 2.66 [27]. Özçelik et al. have simulated laterally and commensurately repeating graphene and boron nitride composite. This nanostructure exhibited resonant tunneling effects [28]. Britnell et al. showed that the resonance through a boron nitride barrier sandwiched between two graphene electrodes occurs when the electronic spectra of the two electrodes are aligned. They observed a strong resonant peak in the current-voltage characteristics of the device with PVRs in the range of 1–4 [29]. The possibility of using graphene nanoribbons in resonant tunneling diodes was investigated by Teong et al., based on using non-equilibrium Green's function with the pi-orbital tight-binding approach. The effects of the graphene shape and the operating temperature on the performance of the device were also investigated. Their results verified that by changing the width and length of the graphene nanoribbons, the resonant tunneling diodes can be tuned for different applications [30].

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In this work, band gap opening in graphene were carried out by making junctions between graphene and graphdiyne nanoribbons. Our results show that graphene-graphdiyne-graphene heterojunctions has non zero band gap and therefore can be used as the channel in resonant tunneling transistors.

## 2. Methods

The atomic and electronic structure calculations were performed using the density functional theory (DFT) approach implemented in the SIESTA code [31]. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) was used to describe the exchange-correlation functional of the electrons. A double-zeta plus polarization (DZP) basis set together with a mesh cuttoff of 200 Ry were adopted for the structures. The brillouin zone k-point sampling was chosen $1 \times 1 \times 5$, based on the Monkhorst-Pack method. The vacuum layers of 20 Å in the non-periodic directions were set to prevent the interaction of adjacent samples. The structure was optimized using the conjugate gradient (CG) algorithm and 0.01 eV/Å maximum force convergence criterions.

The electrical transport properties of the samples were calculated using the TranMain code of OpenMX package through the density functional theory combined with non-equilibrium Green's function (NEGF) formalism [32]. For the transport calculation, the system was divided into three parts: the left electrode (LL), the scattering region (CC) and the right electrode (RR). It was assumed that the electrodes were coupled only with the scattering region, and not with each other. The equation for the Green's function can be written down as:

$$\begin{pmatrix} ES_{LL}-H_{LL} & ES_{LC}-H_{LC} & 0 \\ ES_{CL}-H_{CL} & ES_{CC}-H_{CC} & ES_{CR}-H_{CR} \\ 0 & ES_{RC}-H_{RC} & ES_{RR}-H_{RR} \end{pmatrix} \times \begin{pmatrix} g_{LL} & g_{LC} & g_{LR} \\ g_{CL} & g_{CC} & g_{CR} \\ g_{RL} & g_{RC} & g_{RR} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

that H and S are the Hamiltonian and overlap matrices, respectively. This equation can be solved to calculate the Green's function of the scattering region:

$$g_{CC}(E) = \left( ES_{CC} - H_{CC} - \sum_{L}(E) - \sum_{R}(E) \right)^{-1}$$

The self-energies of the electrodes describe the influence of the electrodes on the electronic structure of the device. Finally, we can define the coupling matrices $\left(\Gamma_{L/R} = i\left(\sum_{L/R}(E) - \sum_{L/R}^{\dagger}(E)\right)\right)$ that allow us to calculate the transmittance of the system for a ballistic process as:

$$T(E) = Tr\left[\Gamma_L g_{CC}^{A} \Gamma_R g_{CC}^{R}\right]$$

If there is no external bias, the transport properties of the system can be obtained as described above. When an external bias is applied on the electrodes, it will only cause a rigid shift of the Eigen values. Conduction in 1D system could be viewed as a transmission problem. The electric current was obtained from the corresponding Green's function and the self-energy by Landauer–Buttiker formula [33,34]:

$$I(V) = \frac{e}{h} \int_{-\infty}^{+\infty} \{T(E,V)[f_L(E,V) - f_R(E,V)]\} dE$$

where $f_L$ and $f_R$ are the Fermi–Dirac distribution functions of the left and right electrodes, respectively.

## 3. Results and discussion

In our previous work [33], the graphene-graphdiyne-graphene (G-GDY-G) heterojunctions with n = 1–4 were studied theoretically. Our results show that the band gap values of G-GDY-G heterojunctions with n = 2–4 are close to zero. So these heterojunctions are not suitable for using as the channel of the nanotransistor.

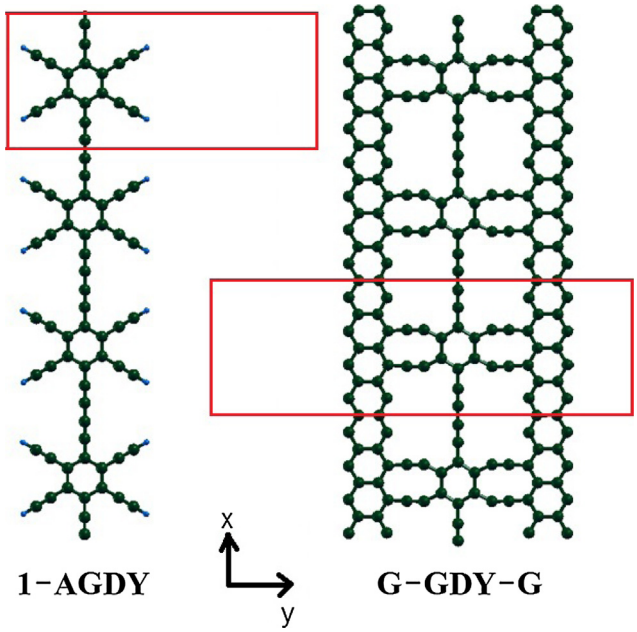


**Fig. 1.** The structure of the 1-AGDY nanoribbon (green color) saturated via Hydrogen (blue color) and G-GDY-G heterojunctions after relaxation. The unit cells are shown with red lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

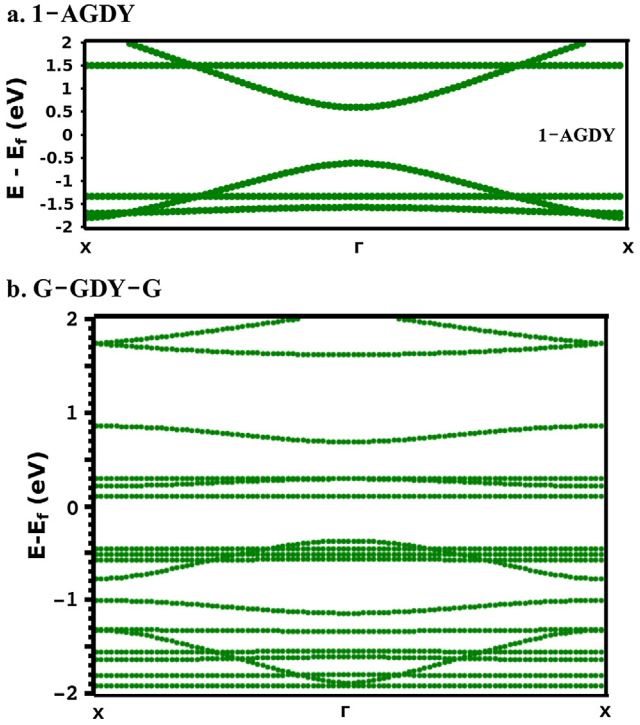


**Fig. 2.** Electronic band structure of (a) 1-AGDY nanoribbon and (b) G-GDY-G heterojunctions.

Therefore, in this work, only G-GDY-G heterojunctions with n = 1 were studied as the channel material.

The armchair graphdiyne with n = 1 (1-AGDY) nanoribbon and graphene-graphdiyne-graphene heterojunctions were first optimized using SIESTA code. Fig. 1 show the structure of the armchair 1-AGDY nanoribbon (green color) saturated via Hydrogen (blue color) and G-GDY-G heterojunctions after relaxation. The band structures are obtained from DFT calculations using the SIESTA package, based on a linear combination of atomic orbital (LCAO) method. Electronic band structure of 1-AGDY nanoribbon and G-GDY-G heterojunctions are shown in Fig. 2a and b, respectively. The Fermi level is set as zero point. Both structures are found to be semiconductors with direct gap at the Γ point in the first brillouin zone. The band gap value of 1-AGDY nanoribbon was obtained $E_g$ = 1.2 eV which larger than that of G-GDY-G heterojunctions (Eg = 0.45 eV).

In order to study the electrical transport behavior of the structures, the current - bias voltage (I-V) curve was computed, using the two probe system. For both systems, the scattering region is connected to the two semi-infinite electrodes of the graphene. The electrical transport occurs along the y direction for both systems. Fig. 3 presents the I-V characteristic of 1-AGDY and G-GDY-G nanoribbons at bias voltages in the range of zero to 2 V. As it can be seen in this figure, below a threshold voltage, the current is almost zero and increases above the threshold voltage. The results indicate that the current in 1-AGDY nanoribbon is larger than that of G-GDY-G heterojunctions. Although the band

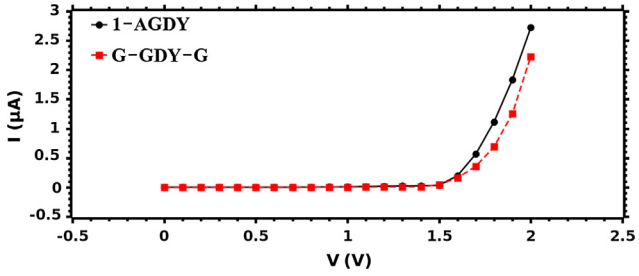


**Fig. 3.** The calculated current of 1-AGDY and G-GDY-G nanoribbons at bias voltages in the range of 0–2 V.

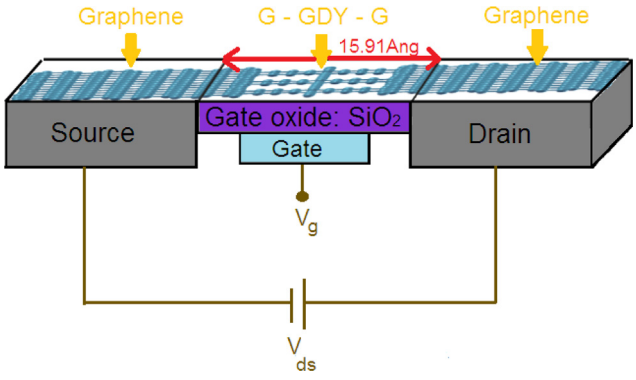


**Fig. 4.** A schematic diagram of G-GDY-G nanotransistor.

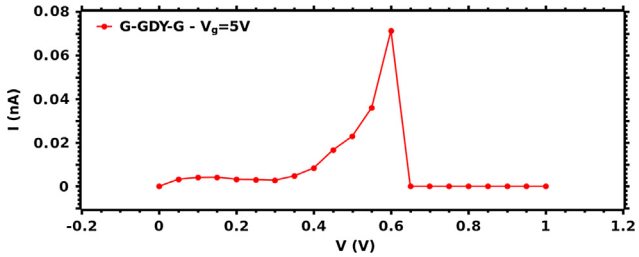


**Fig. 5.** The dependence of the current as a function of the bias voltage at $V_g$ = 5 V and T = 300 K.

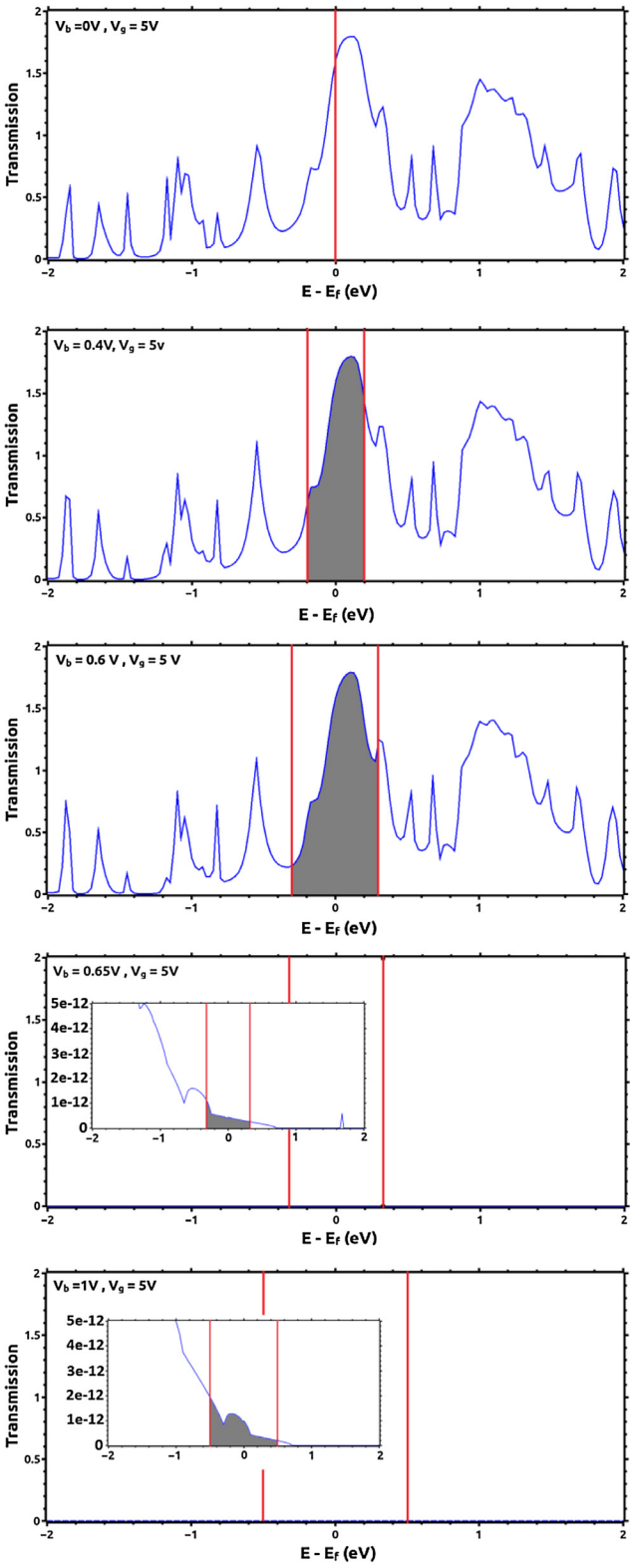


**Fig. 6.** The transmission spectra of the G-GDY-G nanotransistor at bias voltages of 0.0, 0.4, 0.6, 0.65 and 1.0 V.

**Table 1**
Outlined the results of this work and other researches.

| Scatter region | Electrodes | Method | Gate voltage (V) | PVR | Ref. |
|---|---|---|---|---|---|
| G-GDY-G | Graphene | DFT | 5 | 7 | This work |
| Boron nitride | Graphene | Experimental + theoretical | 0, 20 | 1–4 | [29] |
| Boron nitride | Graphene | Experimental + theoretical | −40, 0, +40 | – | [26] |
| GaN-AlGaN | Ga-N | Theoretical (MATLAB) | −1, −2, −3 | 2.66 | [27] |

gap value of 1-AGDY nanoribbon is larger than that of G-GDY-G heterojunctions, its width is smaller which results in fewer electrons scattering process.

Fig. 4 shows a schematic diagram of G-GDY-G nanotransistor. The dependence of the current as a function of the bias voltage at $V_g = 5V$ and $T = 300$ K is given in Fig. 5. The results showed a strong peak at $V_b = 0.6$ V, followed by a region of negative differential conductance (NDC). Other researchers have reported that this peak is attributed to the resonant tunneling of the carriers between the two graphene electrodes [26,29]. When the applied bias voltage is sufficient to lower the energy of an unoccupied quantum state inside the quantum well, to become in the range of source conduction band energy, in this situation it is told that the quantum well is in its resonance state. So the current can pass through the channel and out to the drain. Otherwise, the current is almost zero and the nanotransistor is out of the resonance.

When the bias and gate voltages are set to zero, the chemical potential of the two graphene electrodes is at the Dirac point and the two Dirac points have the same energy. By increasing the bias voltage, electrons and holes accumulate in the negative and positive electrodes respectively, which lead to generation of an electric field, which misaligns the Dirac points. If $V_g \neq 0$, we can adjust $V_b$ to bring the Dirac points of the two electrodes into alignment. Therefore, all the carriers, which have the energies between the chemical potentials of the two electrodes, are allowed to tunnel which resulting a strong peak in the I-V curve.

The transmission spectra of the G-GDY-G transistor at the bias voltage of 0.0, 0.4, 0.6, 0.65 and 1.0 V are presented in Fig. 6. By increasing the bias voltage from zero to 0.6 V, different transmission peaks contribute in the bias window [−eV/2, +eV/2], which are shown by red[1] dashed lines. As a result, the current, which is determined by integrating the transmission function in the bias window, also increases. By rising the bias voltage from 0.6 to 0.65 and 1.0 V, the current decreases abruptly, showing NDC behavior at 0.6 V. The peak to valley ratio (PVR), which is defined as the ratio of the peak current to the valley current, was calculated obtained 7.0 for G-GDY-G transistor. The results obtained in this work as well as the others are outlined in Table 1, for comparison. The obtained PVR value of G-GDY-G heterojunctions is better than boron nitride and GaN. Therefore, this heterojunctions can be suitable for using as the channel in resonant tunneling transistors.

## 4. Conclusion

The resonant tunneling transistors (RTT) are gaining huge interest because of their ability to reduce circuit complexity. The RTT is a very promising candidate in the field of ultra-high speed and ultra-high frequency applications. Due to the dimension reduction down to a few nanometers, quantum effects such as resonant tunneling can occur in G-GDY-G nanotransistors, as is shown in this study. The G-GDY-G nanotransistor is a quantum transport device which produces negative differential conductance (NDC) as well as a high peak-to-valley current ratio (PVR = 7). The resonant conditions exist in a narrow range of bias voltages, which result in a resonant peak in the I-V characteristics, leading to a strong negative differential conductance (NDC).

[1] For interpretation of color in 'Fig. 6', the reader is referred to the web version of this article.

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