**Anabathula Udaya Sri[1*],**

**D. Vinay Kumar[2]**

# Investigating the Transmission Properties, Energy-Momentum Relationship (E-K diagram), and Current-Voltage (I-V) Characteristics of various atomic configurations within Armchair Graphene Nano Ribbons (AGNR) at different bias voltages using the Non-Equilibrium Green's Function Approach

***Abstract:*** - In this research, the investigati on has been done on the behavior of armchair graphene nanoribbons (AGNRs) with 7, 9, and 12-atom when they are subjected to 200,300 and 380 millivolts bias voltages by using Non-Equilibrium Green's Function methodology. The main focus of this research is to study transmission properties, Energy-Momentum (E-K) relationships, and current-voltage (I-V) characteristics. The NEGF method is used to calculate various electronic attributes of AGNRs, including the transmission function, Energy-Momentum (E-K) relationships, and I-V characteristics. Outcomes of this study Explain the interesting factor that with an increasing number of atoms in AGNRs, bandgap decreases. This decrease in bandgap corresponds with an increase in the possibility of transmission in a constrained energy range, which leads to an increase in the device's radius. Because of this, when AGNRs are exposed to a bias voltage, their current flow increases. Additionally, I-V characteristics of AGNRs exhibit nonlinear behavior that becomes stronger as the number of atoms increases and the voltage range increases. Strong electron interactions and the effects of quantum confinement are responsible for this non-linear characteristic. These findings add great significance in advancing the understanding of the electronic properties of AGNRs and offer interesting possibilities for their application in the field of nanoelectronics.

***Keywords:*** Nanostructures, AGNR, NEGF, I-V Characteristics, Transmission, Energy-Momentum (E-K) Diagram

## INTRODUCTION

### AGNRs

Because of AGNRs' unique electrical, mechanical, and thermal properties, graphene nanoribbons (GNRs) have attracted a lot of attention and have been considered highly attractive possibilities for future nanoelectronics applications. Armchair graphene nanoribbons (AGNRs) are one of the many types of GNRs, and they have shown extraordinary electrical properties. AGNR transport properties have been studied utilizing several theoretical approaches. However, the transport behavior of non-equilibrium AGNRs under the influence of voltage remains an area that has not been thoroughly investigated.

Previous studies have demonstrated that Armchair Graphene Nanoribbons (AGNRs) have defined bandgap and unique edge states [1, 9], which significantly impact their electrical properties Further, AGNRs' bandgap has shown by theoretical calculations, can be changed by adjusting their edge arrangement [2-4, 10] and width.

In addition, it has been shown that the electrical characteristics of AGNRs are noticeably sensitive to faults [11–13]. However, an extensive investigation of the methods in which faults affect the transport characteristics of AGNRs whenever bias voltage is applied is still a topic that needs more research.

### NEGF Method

One powerful theoretical technique for exploring the electrical properties of nanoscale structures, such as quantum dots, nanowires, and graphene nanoribbons, is the Non-Equilibrium Green's Function approach. This technique gives a structured approach to investigating transport characteristics of non-equilibrium systems when bias voltage is applied, which is an essential component for understanding how effectively they function

[1*,2]Vignan's Foundation for Science, Technology and Research, Vadlamudi, Andhra Pradesh- 522213, India
*Corresponding Author: Anabathula Udaya Sri

Email:- udayasrivfstr@gmail.com

in nanoelectronics devices.

The NEGF method is Green's function formalism, a framework for explaining how a system behaves about external perturbation. The system's electronic structure is defined by its Hamiltonian in this technique, and under non-equilibrium conditions, the Green's function equations of motion are solved to analyze the transport properties. This technique is applied for a broad range of research on electrical properties, including evaluation of noise, current-voltage(I-V) characteristics, and transmission in nano-scale systems. Moreover, it has shown to be extremely useful in investigating how disorder, interactions, and other variables affect these systems' electrical properties.

The NEGF technique has been widely used in many different kinds of nanoscale systems. Furthermore, the technique has shown promise in investigating transport features in more complex systems, including topological insulators [15–17] and molecular electronics [12–14].

This work investigates Armchair Graphene Nanoribbons (AGNRs) in detail, concentrating on their energy-momentum (E-K) characteristics, current-voltage (I-V) profiles, and transmission attributes. The analysis used in the study makes use of the powerful Non-Equilibrium Green's Function approach. This research significantly expands comprehension of Armchair Graphene nanoribbons, probing transport behaviors, Energy-Momentum (E-K) relationships, and I-V attributes of AGNRs composed of 7, 9, and 12 atoms. These AGNRs are subjected to bias voltages of 200 mvolts, 300 mvolts, and 380 mvolts, and their electronic properties are evaluated using the NEGF method. The results obtained from this study provide new perspectives on the transport behavior of AGNRs when bias voltage is applied. These results could direct the development of future nanoelectronics devices, offering possibilities to creative discoveries in this area.

**METHODOLOGY**

The process for investigating the Energy-Momentum Relationship (E-K diagram), Transmission properties, and I-V characteristics of Armchair Graphene Nano Ribbons through the application of Non-Equilibrium Green's Function includes various steps, as mentioned here.

The first step is to use the tight-binding Hamiltonian to model the Armchair Graphene Nano Ribbon (AGNR). This Hamiltonian takes these interactions into account Concerning the nearest-neighbor relationships among the carbon atoms in the graphene lattice. The scattering area is then built using the Hamiltonian which is composed of AGNR connected to semi-infinite leads. Electrodes for the source and drain are represented by these leads. It's important to remember that in this investigation, we assume that graphene makes up both leads, similar material as the AGNR channel.

The equations for Non-Equilibrium Green's Function (NEGF) have to be derived in the second phase. These formulas are generated by combining self-energy functions that describe leads with the Hamiltonian. These self-energy functions describe the relationship between the electrodes and the scattering region. After that, utilizing these iterative Green's function techniques, the NEGF equations are solved numerically. Armchair Graphene Nano Ribbon's (AGNR) transmission attributes and current-voltage (I-V) characteristics are provided to us by this solution.

The third step involves verifying the correctness of the NEGF methodology by contrasting the outcomes with those generated by applying different theoretical methods, like Density Functional Theory (DFT) and the Landauer-Büttiker formalism.

Finally, investigation of the effects of various parameters such as the width, length, voltage, temperature, and doping level of AGNR electronic characteristics. It is important to remember, that the main focus of this work remains on analyzing the energy-momentum (E-K), current-voltage (I-V), and transmission properties exhibited by AGNRs with 7, 9, and 12 atoms at different bias voltages, notably 200 mV, 300 mV, and 380 mV, of AGNRs. A list of equations that are essential to this investigation can be seen below.

Expression for the calculation of quantum wave (Ψ) for any type of particle such as an electron (Schrodinger equation)

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t)=\left[\frac{-\hbar^2}{2m}\nabla^2+V(r,t)\right]\Psi(r,t)\ (1)$$

Expression for the calculation of quantum wave (Ψ) for Time Independent particle (Time-Independent Schrodinger Equation)

$$\left[\frac{-\hbar^2}{2m}\nabla^2+V(r)\right]\Psi(r)=E\Psi(r)\ (2)$$

Expression for the calculation of quantum wave (Ψ) for free electrons

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(r)=E\Psi(r)\ (3)$$

By solving he above obtained equation here gets the function

$$\Psi=A\cos\left(\frac{2\pi}{\lambda}x\right)(4)$$

Expression for Green's Function

$$G(E)=x(EI-H-\Sigma_L-\Sigma_R)^{-1} \qquad (5)$$

Expression for the calculation of current in the channel

$$I_{LR}=\int_{-\infty}^{\infty}\frac{e}{h}T(E)(f_L-f_{\square})dE \qquad (6)$$

Expression for fermi-level energy

$$f=\frac{1}{1+e^{\frac{E-E_F}{kT}}} \qquad (7)$$

Expression for transmission property

$$T(E)=\tan(\Gamma_L G(E)\Gamma_R G^*(E)) \qquad (8)$$

Expression for Green's Function

$$G(E)=x(EI-H-\Sigma_L-\Sigma_R)^{-1} \qquad (9)$$

Expression for self-energy

$$\Sigma=\tau g\tau^+ \qquad (10)$$

**E-K Diagram For Free Electron**

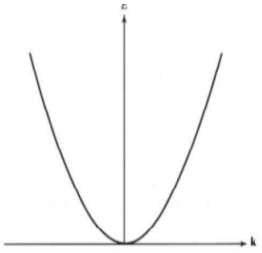


**Fig.1 E-K diagram for free electron**

E = energy of an electron, K = wave vector, for free electron the Potential Energy is zero

K.E + P.E = T.E, Hence K.E = T.E

$$E = \frac{h^2 k^2}{2m} \quad (11)$$

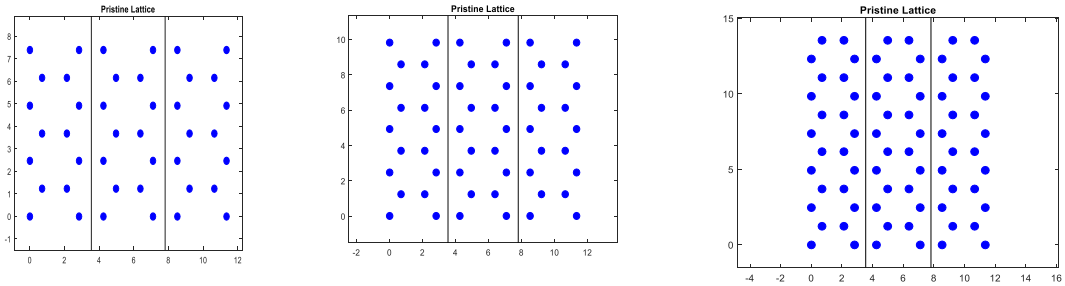
Fig. 1 shows how the energy and speed of electrons relate to each other when the free electrons' wave vector (K) varies from "0" to "∞." As a result, there is a change in energy (E) from "0" to "∞." The Energy-Momentum (E-K) diagram is a graphic representation that shows the permissible energy levels and the corresponding momentum of electrons at particular energy states. The material's structural makeup is further described by the E-K diagram, which shows whether the material acts like a semiconductor or a metal. This representation also can identify band gap is direct or indirect. Extracting the band gap from the E-K diagram is one approach, but it can also be determined using the electronic properties of the material. Simplifying the time-independent equation helps to achieve these realizations.

$$H\Psi = E\Psi \quad (12)$$

where H=Hamiltonian operator (energy operator) and E=Energy eigen value.

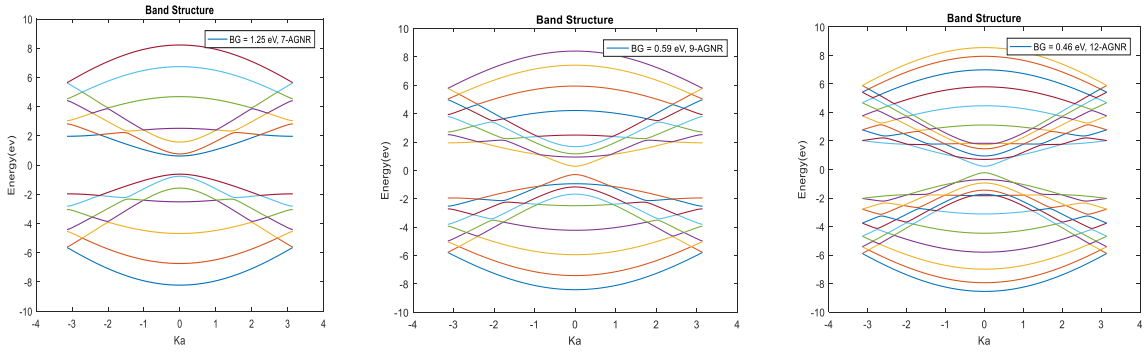
## RESULTS AND DISCUSSION

In this particular section, findings of the conducted study on pristine lattices are given. Fig. 2 demonstrates the atoms' arrangement in the chosen 7,9,12-atom AGNR in a honeycomb structure. The AGNR widths in this structure are 0.74 nm, 0.98 nm, and 1.25 nm for the 7, 9, and 12-atom AGNRs, respectively. From that observed that as no. of atoms increases in the honeycomb structure the width increases consequently resulting in an expansion of the device's radius




**7-AGNR** **9-AGNR** **12-AGNR**

**Fig. 2 Pristine lattice of 7, 9, 12-AGNR honeycomb structure**




**7-AGNR** **9-AGNR** **12-AGNR**

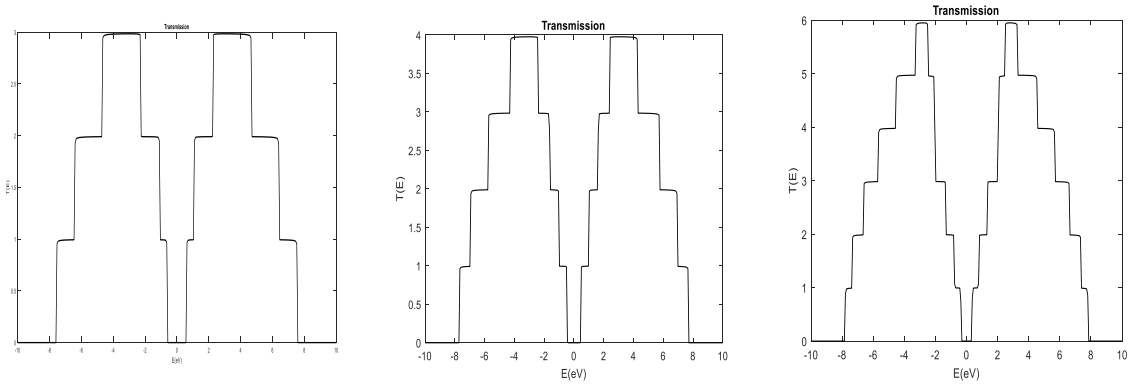
**Fig. 3 Energy-Momentum (E-K) Diagrams of 7,9,12- atom AGNR**

The band structure, shown as an Energy-Momentum (E-K) diagram, for 7, 9, and 12-atom Armchair Graphene Nanoribbons (AGNRs) with armchair edges are shown in Fig. 3. Two different bands are shown in this diagram, spaced apart by a band gap. The upper set contains conduction bands, conduction bands are not

occupied by electrons, and the valance bands in the lower set are entirely occupied by electrons. For 7, 9, and 12-atom AGNRs, the band gap values are 1.25 eV, 0.59 eV, and 0.46 eV, respectively. This band gap gives the energy required to move an electron from the valence band to the conduction band, defining the AGNR's electrical properties.

For AGNRs with a width of 7, 9, and 12 atoms and armchair edges, band structure shows a band gap, setting them apart from their more extensive counterparts. When materials are sized down to the nanoscale, quantum confinement phenomena occur, leading to this band gap. When it comes to AGNRs, the observed band gap results from a reduction in the accessible states caused by the confinement of electrons and holes along the ribbon's width.

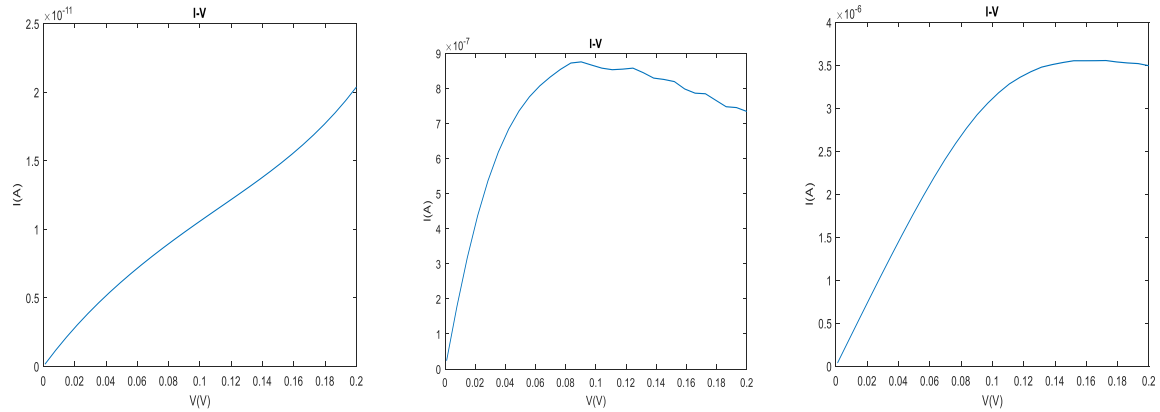
Additionally, the band gap appears to narrow with increasing atomic number, indicating a decrease in the energy needed to move an electron from a valence band into a conduction band.




**7-AGNR** **9-AGNR** **12-AGNR**

**Fig. 4 Transmission of 7, 9, and 12-atom AGNRs**

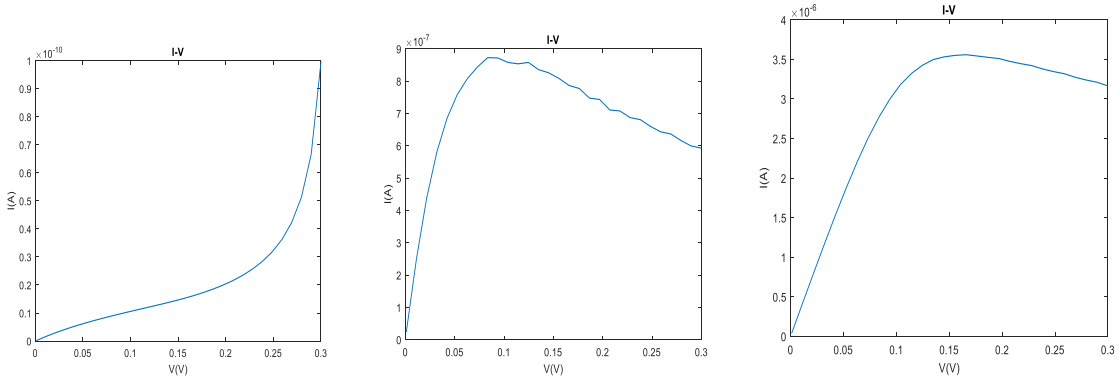
The Transmission-Energy diagram, shown in Fig. 4, provides crucial insights into the electronic properties of 7, 9, and 12-atom-wide Armchair Graphene Nanoribbons (AGNRs) across an energy range spanning from -10 eV to +10 eV. The distinctive shape of this diagram depends on several factors inherent to AGNR, comprising its measurements, degree of doping, and temperature. The transmission energy diagram of AGNR shows a nonlinear relationship between momentum, and energy, spanning an energy range of -10 eV to +10 eV. The energy eigenvalues present in the structure cause an electric field to be generated across the AGNR, which in turn causes changes in the energy levels of the holes and electrons. This is the reason for the non-linearity. Significantly, this occurrence is correlated with the band gap's reported decrease with increasing atomic number, which suggests that less energy is needed to move an electron from a valence band to a conduction band.




**7-AGNR** **9-AGNR** **12-AGNR**

**Fig. 5 I-V Characteristics of 7, 9, and 12-atom AGNRs under a bias voltage of 200 mV**

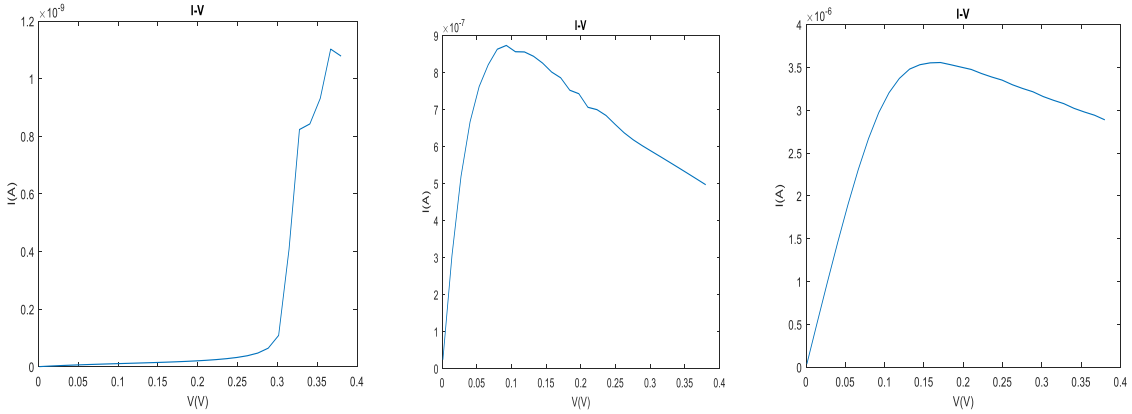
Fig. 5 illustrates for 7, 9, and 12-atom AGNRs, how current flowing through the device increases quickly from zero when bias voltage 200 mV is applied, ultimately reaching saturation point, when the flow of current stops and remains constant. After reaching the point of saturation, it can be observed a drop in current in the I-V curve for 9 and 12-atom AGNRs. All of the I-V trends in Fig. 5 exhibit a steeper I-V curve and a greater saturation current, which are attributed to either a reduced band gap or a higher carrier concentration in the structure.




**7-AGNR** **9-AGNR** **12-AGNR**

**Fig. 6 I-V Characteristics of 7, 9, and 12-atom AGNRs under a bias voltage of 300 mV**

Fig. 6 illustrates the behavior of current through the Armchair Graphene Nanoribbons (AGNRs) under a bias voltage of 300 mV. As voltage is applied, the current initially surges rapidly from zero for the 7-atom AGNR. However, for the 9 and 12-atom AGNRs, there is an initial increase in current until it reaches a saturation point. Similar to the previous case, the available conducting states within the AGNRs determine this saturation current. Following the saturation point, a decrease in current or a decline in the I-V curve is observed for the 9 and 12-atom AGNRs. This pattern is in consistent with the steeper I-V curve and deeper saturation current exhibited in all of the I-V charts shown in Fig. 6. This effect is explained by either a smaller band gap or a higher carrier concentration inside the structure.




**7-AGNR** **9-AGNR** **12-AGNR**

**Fig. 7 I-V Characteristics of 7, 9, and 12-atom AGNRs under a bias voltage of 380 mV**

Fig. 7 offers a thorough understanding of the current behavior of Armchair Graphene Nanoribbons (AGNRs) when subjected to a bias voltage of 380 mV. Upon the application of voltage, the current initially undergoes a rapid surge from zero for the 7-atom AGNR. For the 9 and 12-atom AGNRs, there is an initial increase in current until it reaches a saturation point, as previously discussed. This saturation current is dependent on the availability of conducting states within the AGNRs. Subsequently, beyond the saturation point, there is a

noticeable decline in current or a decrease in the I-V curve for the 9 and 12-atom AGNRs. All of the I-V graphs in Fig. 7 show a continuous trend of a steeper I-V curve and a greater saturation current. This is explained by either a narrower band gap or an elevated carrier concentration within the structure. These two aspects are consistent with the growing number of atoms in the AGNRs

## CONCLUSIONS

In this work, investigation has been done on the energy-momentum (E-K), current-voltage (I-V), and transmission properties exhibited by Armchair Graphene Nanoribbons (AGNRs) with 7, 9, and 12 atoms. These AGNRs were subjected to bias voltages of 200 mV, 300 mV, and 380 mV, and our investigation was conducted employing the Non-Equilibrium Green's Function (NEGF) methodology.

Our research has brought illumination to several significant components of AGNR behavior. First, we noticed that the width of the AGNR expands in proportion to the number of atoms in the honeycomb structure, which eventually leads to a bigger device radius. It also discovered that the band gap decreases with increasing atomic number in the AGNR, indicating a decrease in energy needed to move an electron from a valence band to a conduction band.

Results discovered that AGNR coefficient transmission increases as the atom number increases, reaching a maximum at the Fermi energy. This observation strongly suggests the conductivity characteristics of AGNRs are strong. It has observed variations in terms of the I-V characteristics at different bias voltages.

The I-V curve for 7-atom AGNRs showed a linear connection between current and voltage at a bias voltage of 200 mV, suggesting Ohmic behavior. However, under bias voltages of 300 mV and 380 mV, as voltage is applied, the current initially surges rapidly from zero. In contrast, for the 9 and 12-atom AGNRs at bias voltages of 200 mV, 300 mV, and 380 mV, an initial increase in current occurs until it reaches a saturation point. The presence of conducting states within AGNRs determines this saturation current. Following this saturation point, a noticeable decrease in current or a decline in the I-V curve becomes evident. This consistent behavior reinforces the role of available conducting states within the AGNRs in determining the observed saturation current, followed by the subsequent reduction in the I-V curve.

Ultimately, this work shows how useful the NEGF approach is for investigating the electrical characteristics of AGNRs. The results of this study may affect future AGNR-using electronic product designs. To completely understand the electrical properties of AGNRs and create useful applications for these extraordinary materials, more study in this area is required.

## REFERENCES

[1] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Nonequilibrium Problems, *Addison-Wesley Publishing Company* (1962).

[2] Meir, Yigal, and Ned S. Wingreen. Landauer formula for the current through an interacting electron region. *Physical review letters* 68.16 (1992): 2512.

[3] Ferry DK, Goodnick SM. *Transport in Nanostructures*, Cambridge Univ. Press, Cambridge 1997.

[4] Szałowski K. Graphene nanoflakes in external electric and magnetic in-plane fields, *Journal of Magnetism and Magnetic Materials*. 2015 May 15;382:318-27.

[5] Cai J, Ruffieux P, Jaafar R, Bieri M, et al. Atomically precise bottom-up fabrication of graphene nanoribbons. *Nature*. 2010 Jul 22;466(7305):470-3.

[6] Sadeghi MM, Pettes MT, Shi L. Thermal transport in graphene. *Solid State Communications.* 2012 Aug 1;152(15):1321-30.

[7] Yin, Yiheng, Zhaofu Zhang, et al. Tellurium nanowire gate-all-around MOSFETs for sub-5 nm applications. *ACS Applied Materials & Interfaces* 13, no. 2 (2021): 3387-3396.

[8] Zhou, Min, Hao Jin, et al. In-plane dual-gated spin-valve device based on the zigzag graphene nanoribbon. *Physical Review Applied* 13, no. 4 (2020): 044006.

[9] Son, Young-Woo, Marvin L. Cohen, et al. Energy gaps in graphene nanoribbons. *Physical review letters* 97, no. 21 (2006): 216803.

[10] Wakabayashi, Katsunori, Yositake Takane, et al. Edge effect on electronic transport properties of graphene nanoribbons and presence of perfectly conducting channel. *Carbon 47, no. 1* (2009): 124-137.

[11] Li, Xiaolin, Xinran Wang, Li Zhang, Sangwon Lee, et al. Chemically derived, ultra-smooth graphene nanoribbon semiconductors. *science 319*, no. 5867 (2008): 1229-1232.

[12] Yang, Siqi, Daixin Li, Tianran Zhang, et al. First-principles study of zigzag MoS2 nanoribbon as a promising cathode material for rechargeable Mg batteries. *The Journal of Physical Chemistry* C 116, no. 1 (2012): 1307-1312.

[13] Kim, Hee Jin, Ho Young Kim, et al. Recent advances in non-precious group metal-based catalysts for water electrolysis and beyond. *Journal of Materials Chemistry* A 10, no. 1 (2022): 50-88.

[14] Wu, Qingyun, Lei Shen, et al. Electronic and transport properties of phosphorene nanoribbons. *Physical Review* B 92, no. 3 (2015): 035436.

[15] Wakabayashi, Katsunori, et al. Electronic transport properties of graphene nanoribbons. *New Journal of Physics* 11, no. 9 (2009): 095016.

[16] Li, Dongde, Di Wu, Xiaojiao Zhang, et al. The spin-dependent electronic transport properties of M (dcdmp) 2 (M= Cu, Au, Co, Ni) molecular devices based on zigzag graphene nanoribbon electrodes. *Physics Letters* A 382, no. 21 (2018): 1401-1408.

[17] Zhang, Peina, Xinlu Li, et al. π- magnetism and spin-dependent transport in boron pair doped armchair graphene nanoribbons. *Applied Physics Letters* 120, no. 13 (2022): 132406.