A Novel Graphene Modelling: Bottom up Approach - Band Gap Studies to Transport in Python

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Research Article

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A Novel Graphene Modelling: Bottom up Approach - Band Gap Studies to Transport in Python

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Abstract. In this work we develop a computational, quantum level monolayer graphene nanoribbon (GNR) MOSFET of channel length of 10 and 20 nm, with a width of 2 nm and contacts of 2nm width is attached. To develop the MOSFET channel, a bottom up approach is adopted by developing the material model. First the material models of graphene nanoribbon is developed using pybinding module tool in python. The material models of monolayer, bilayer graphene nanoribbon are built on the principles of tight binding module. The methodology developed is based on the Hamiltonian matrix formulation that has been used to determine the E-k plots and LDOS plots of graphene monolayer, bilayer graphene nano ribbon. The GNR MOSFET that is structurally built in python is used to simulate graphene as a switch. Its band gap characteristics is presented as its performance as a switch and is verified with relevant work. Then GNR MOSFET is modelled using quantum principles of NEGF and greens function to determine the transmission characteristics and the I-V characteristics for channel lengths of 10 nm and 20 nm.

Keywords: Tight binding modelLAPACKPythonNEGFQuantum nano devicesGraphene Nanoribbon(monolayer, bilayer)MOSFET

1 Introduction- Graphene, Modeling and Applications

The scaling of feature sizes of silicon-based semiconductors and MOSFETs into nanoscale range will not be possible indefinitely due to the deep submicron effects and tunneling effects. Deep submicron effects and tunneling effects have been mitigated to some extent using the principles of channel engineering as in FINFETs and allied devices. These effects at nanoscale on semiconductor MOSFETs have been analyzed by development of quantum principles. It is required that quantum studies are to be undertaken from molecular principles. So the motivation here is to develop the bottom up approaches from molecules to devices to study the bandgap and present the transport characteristic of MOSFET channel built of graphene nanoribbon. Graphene based material devices are being explored as potential non-silicon materials ever since graphene which was

isolated in 2004[1].
The semiconductor technology roadmap had recommended the integration of graphene material in future semiconductor devices due to the availability of graphene in the form of large-area sheets and its ultra-high carrier mobility. Although the use of graphene as channel material would have several advantages, the development of graphene or graphene nano ribbon FETs is challenging because of the lack of a sizeable bandgap [2][3][4][5]. The lack of band gap is more of a hurdle mainly in logic devices that require a reduced off current than in analog devices that are used in radio frequency applications [7]-[9]. The properties of graphene show that it is a semimetal in which the valence and the conduction band meet or overlap and the charge carriers have zero effective mass [10][11][12]. Graphene has shown great promise due to its various inherent properties like better thermal conductivity, good mechanical strength, higher mobility at room temperature, making its use in building faster and smaller transistors [13]. Additionally, its ability to handle terahertz frequency makes it possible to fill up the terahertz gap, and hence it is a potential candidate for MOSFET channel material [14]. Tuning the bandgap of graphene to increase on/off current ratio is the key of success for it to be used as a channel material in MOSFET transistors[15]. The tight binding methodology has been widely applied to the study of the energy band structure of graphene and other two-dimensional materials. pybinding tools are incorporated in python libraries [16]. Quantum tunneling in tunneling MOSFETs and study of sensors based on bottom up approaches have used tight binding models [17]. Also the tight-binding calculations have been used to analyse the transport features and to understand the origin of the various modes of transport in graphene nanoribbons using full-scale quantum-transport simulations [18]-[21].
Graphene material also has been used to develop digital logic to build boolean gates. The digital characteristic requirements have been explored and modelled using the non-equi-
librium Green's function and Landauer formalism. Also, graphene has been explored for its usage as a digital switches as there is a huge demand for devices that function as components for large-scale digital circuits[22],[23]. Coming back to transport in graphene channel based MOSFETs, mode space approach has been used to develop transport computations of carriers to determine the current using NEGF which is computationally extensive [22]-[25].
Stacks of graphene built of monolayer and bilayer graphene were modelled as R-L-C circuits to study the variation of the input impedance, absorbance, reflection coefficient and absorption frequency with respect to the variation of thickness of the dielectric layer[26]. Various compact models and computation of quantum capacitances has been carried out to simulate circuits of graphene MOSFETs [27]-[29]. Gate all around MOSFET circuits of numerical models developed and been validated with ATLAS TCAD simulation for implementing the device as an inverter circuit and gain value is also estimated [30]. Graphene has a lot of futuristic applications and methods to determine the various parameters have been adopted for successful modelling of the material [31]-[33].

The focus here is to develop a graphene nanoribbon MOSFET (GNR MOSFET) transistor by using bottom up approach from molecule to material. The aim of the work is to present it as a model development from material to device. The first step towards this is to simulate the band gap properties of the structure built with graphene material of monolayer, bilayer and graphene nano ribbon. The band gap properties are simulated using tight binding model which is used in the formulation of the Hamiltonian that is used in plotting the energy in the band gap. Further, graphene nanoribbon based channel is used in MOSFET to study the transport properties using non-equilibrium greens function (NEGF) to account for the I-V characteristics of graphene MOSFETs. Also a graphene nanoribbon based MOSFET switch is developed in python with source, drain, gate contacts and results of GNR MOSFET and switch is presented. The state of art in graphene transport is discussed in section 2. Section 3, discusses the relevant theory for molecular representation. The results are presented in section 4 and 5 using plots of eigen values and band structure. Finally transport of carriers is studied to bring out the current versus voltage in graphene channel based MOSFET.

2 Graphene Material from first principles

The basic relationship between the carriers namely electrons and their occupancy at various energy levels is revisited here. The energy level at which an electron finds itself in any material as treated by the wave particle theory is symbolically expressed as ψ. The current density J is defined by expression (1).

$$J = Re[\frac{-i\hbar}{m}\psi * \nabla\psi] \tag{1}$$

J is determined by standard Schrödinger's wave equations, where herein time-independent Schrödinger equation (single nonrelativistic particle) is considered,

$$\nabla^2\psi = \frac{-2m}{\hbar^2}[E-U]\psi \tag{2}$$

where ∇^2 is the space operator in one, two or three dimensions as applicable to the plane or space of the device and

$$k^2 = \frac{2m}{\hbar^2}[E-U] \tag{3}$$

The wave function is represented in Bloch form in continuous integral form as in expression(4)

$$\varphi(ax) = \sum_j e^{i\frac{2\pi n}{N}j}\emptyset(ax - jat_o) \tag{4}$$

And further as a linear summation form over all lattice vectors At as in expression (4) and (5)

$$\varphi(ax) = \sum_R e^{iK.At}\emptyset(ax - At) \tag{5}$$

Under Hückle/tight binding approximations, The LHS of the above equation expands as given below in expression (6) [17][22],

$$\langle \emptyset_1(At)|H|\varphi(ax)\rangle = \big(c_1\alpha + c_2\beta(1 + e^{-ik\bar{a}x_1} + e^{-ik\bar{a}x_2})\big)e^{ik.At}$$

$\langle \emptyset_2(At)|H|\varphi(ax)\rangle = \big(c_2\alpha + c_1\beta(1 + e^{-ik\bar{a}x_1} + e^{-ik\bar{a}x_2})\big)e^{ik.At}$(6)
and RHS expands to,

$$\varepsilon\langle \emptyset_1(At)|\varphi(ax)\rangle = \varepsilon c_1 e^{ik.At}\varepsilon\langle \emptyset_2(At)|\varphi(ax)\rangle = \varepsilon c_2 e^{ik.At} \tag{7}$$

The solution for $c1$ and $c2$ is given by

$$\begin{vmatrix} \alpha - \varphi & \beta(1 + e^{-ik\bar{a}x_1} + e^{-ik\bar{a}x_2}) \\ \beta(1 + e^{-ik\bar{a}x_1} + e^{-ik\bar{a}x_2}) & \alpha - \varphi \end{vmatrix} = 0$$

$$\implies \varepsilon = \alpha \pm \sqrt{3 + 2cos(k.\bar{a}x_1) + 2cos(k.\bar{a}x_2) + 2cos\big(k.(\bar{a}x_1 - \bar{a}x_2)\big)}(8)$$

2.1 Solving the Hamiltonian to plot the E-k Diagram

The Hamiltonian is formulated for the Hamiltonian operator. The Hamiltonian in the matrix form of the type shown in expression (9) represents the on-site potential at different lattice corners. The general Hamiltonian matrix for a 1-D chain of the material structure is given as the matrix in expression (9).Each atomic site is related to its nearest neighbour by t , and 2t for a site that has atoms on both its side in a 1-D linear chain, where is the hopping parameter between two neighbour atoms in the 1-D chain. The Hamiltonian is solved to determine the eigen values using the methodology as described by the flow chart.

$$H = \begin{vmatrix} ... & t & 0 & 0 & 0 & 0 \\ t & 2t & t & 0 & 0 & 0 \\ 0 & t & 3t & t & 0 & 0 \\ 0 & 0 & t & 2t & t & 0 \\ 0 & 0 & 0 & 2t & t & 0 \\ 0 & 0 & 0 & 0 & t & 2t \end{vmatrix} \qquad [22][24] \tag{9}$$

2.2 Python and Pybinding

Python is a interpreter based computer programming language. It provides a large set of libraries and modules for tight binding calculations in atomic structures, two of which are Pybinding[16] and Kwant[33]. The pybinding library in python provides a material repository which includes graphene, making it easier to design Graphene lattices of varying structure, and energy. Here we use pybinding for computing atomic structure of graphene monolayer, bilayer and graphene nanoribbon and Kwant module of python for solving the Green's Function to obtain the transport characteristics to plot the IDS versus VDS characteristics of Graphene MOSFET.

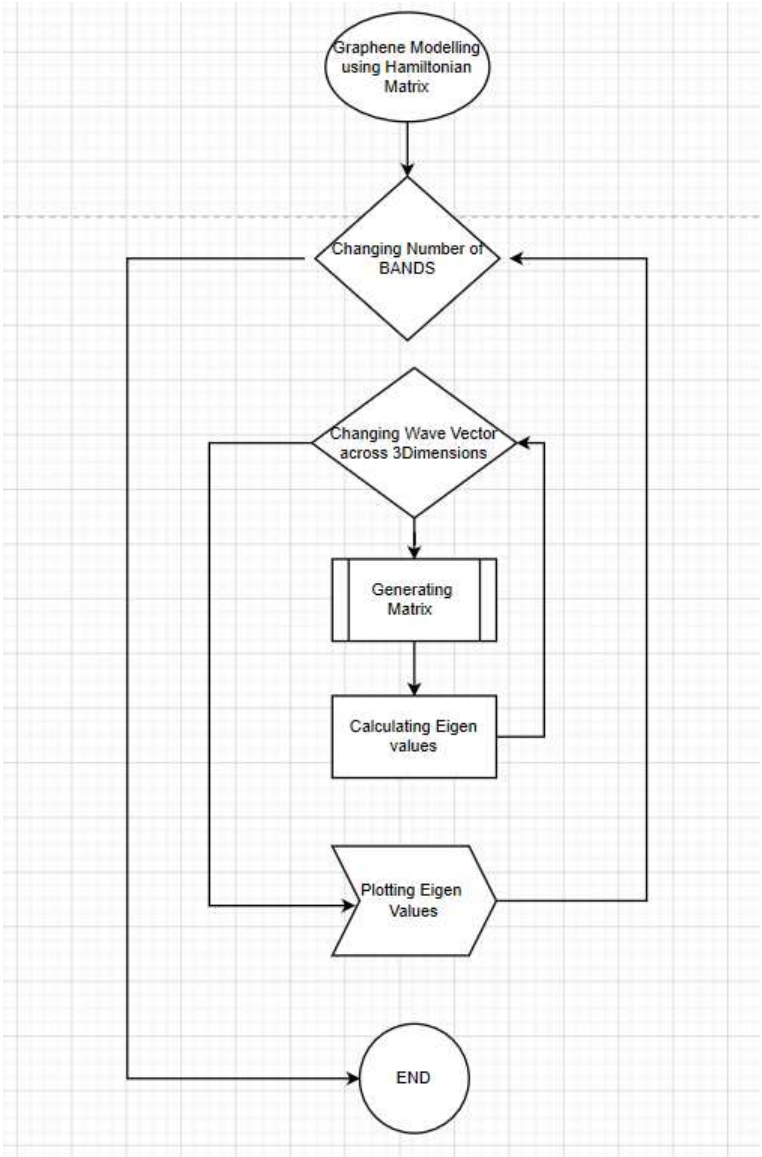
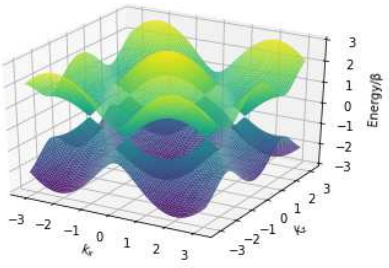


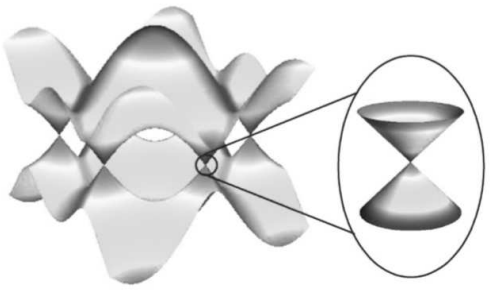
Fig. 1: Flowchart for E-k diagram of plots in Figure.

2.3 Role of pybinding in energy plots

We start with a graphene 2-D structure, and solve the Hamiltonian matrix across two-dimension, x and y as explained in the methodology using the flowchart in Figure 1. As the number of points along are increased, the energy curves become smoother and the computation required increases.
The flowchart in Figure 1 gives the methodology as the flow of computer algorithm to solve for the Hamiltonian matrix given from expressions (9). Since pybinding is not very computationally demanding, it is easily executed on standard personal computers. Figure.2 shows the plotting of Graphene in 3D in python. The energy bands are extracted using the methodology described in Figure.1 and plotted from expression (9) in Figure.2a. The plot is similar with the plot in Figure.2b [23], used for corroborating the 3-D graphene E-k diagram developed in python. The plot in Figure.2a are the plots of the energy bands of graphene obtained using the tight binding model, the energy points are zero where the bands meet and are termed the dirac points or K points, also defined as Brillouin zone[32].

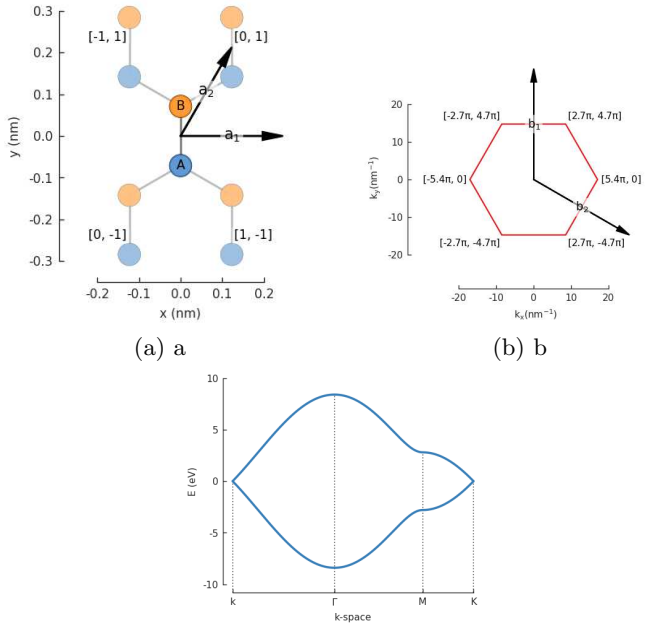


(a) a



(b) b

Fig. 2: (a) Performance comparison python approach and graphene 3D plot (b) Band structure of graphene[23].



(a) a (b) b

(c) b

Fig. 3: (a) Monolayer Graphene Lattice structure (b) Monolayer Graphene Brillouin Zone (c) E-k Graph Monolayer Graphene

3 Graphene lattice, Brillouin Zone, E-k Graph Monolayer Graphene- 2-D structure

The development of the simulation starts with building a model of monolayer graphene (available in Pybinding repository of materials) with translational symmetry. Pybinding supports various Solvers such as LAPACK – a standard software library for solving linear algebra for eigen values, eigen vectors and decomposition, ARPACK- written in Fortran 77 for solving large eigen value problems. The structure of Graphene Lattice is plotted using Pybinding. Pybinding allows us to plot the brillouin layer, E-k plot and the Local Density of states(LDOS) using built-in functions. The lapack solver is used, which gives the eigen values of the graphene structure necessary to form the Hamiltonian Matrix. Next the limits are fixed using the graphene material properties such as unit cell length. Once the limits have been calculated the eigen values are found for both the upper band and lower band.

3.1 Graphene Monolayer

The Graphene monolayer is structured by setting the wave vector for the material, calculated initially, followed by storing the eigen values in an empty list. These eigen values are then plotted together to give the E-k plot of Graphene.

Using the Pybinding library in Python[16], which provides functions to calculate the Hamiltonian, the Graph is obtained for Monolayer Graphene structure in Figure 3a, Brillouin Zone in Figure 3b. and E-k plot in Figure.3c.

The detailed methodology adopted to obtain the monolayer graphene structure, its Brillouin Zone and its E-k plots is explained and elaborated in the Figure 4.

Steps for Constructing Graphene Monolayer Structure (Or any Graphene Structure)

1. Import Graphene Repository from Pybinding, Pybinding has material repository for Graphene, Phosphorus and Group 6 TMDs.
2. Define Shape of the structure. Shape can be defined using pre-built function or using custom functions as show in code below.
3. Define Graphene model using Type (Monolayer, Bilayer, used to define Lattice), shape and Symmetry and comile the model.
4. Plot the model using the plot function in Pybinding.
5. To plot the Brillouin Zone of Graphene, the lattice alone is imported and the Brillouin Zone is plotted using the plot_brillouin_zone() property of the Lattice class available in Pybinding.
6. To calculate the Hamiltonian and Band-structure of the compiled model (Step-3). Pass the model through a solver, the eigen solvers avaiable in Pybinding are LAPACK, ARPACK.
7. The output from this solver is used to calculate the bands and local density of states.
8. The Band plot is plotted using the returned Band output from the solver.calc_bands function.
9. The LDOS plot is plotted using the returned Band output from the solver.calc_bands function.

Fig. 4: Methodology for Graphene monolayer

Figure.5 shows the plot of Monolayer Graphene with its corresponding Brillouin layer, E-k diagram and Local Density of states (LDOS) plot.

3.2 Graphene Nano ribbon lattice, Brillouin Zone, E-k Graph Graphene Nanoribbon

The methodology in Figure.4, is extended to create graphene nano ribbons(GNR) structure and lattice, plotted in Figure 6. The same is run in python to plot the band structure of GNR for zig-zag and armchair structures. The E-k diagram and LDOS plots of GNR is obtained in Figure 6.(b) and (e). This shows that the band structure of Graphene changes with varying structures of graphene, when compared to plots of Figure.5 and Figure 3.

3.3 Graphene Bilayer Nanoribbon Lattice, Brillouin Zone, E-k Graph

The uniqueness of Graphene is not limited to only its semi metal properties, but also its bilayer structure. Again Pybinding provides functions to easily plot the bilayer graphene. Like the Graphene Monolayer Nanoribbon, a Graphene Bilayer Nanoribbon can be plotted as seen in Figure 7.

4 Graphene Nanoribbon as a Switch

Pybinding can also be used to model graphene as a switch. The architecture of the switch modelled in this paper is as proposed by [21]. A semiconducting Arm chair GNR is connected to left and right graphene leads, here the leads will be referred to as lead0 on the left hand side and lead1 on the right hand side. Figure N shows the proposed graphene switch. This work will now aim to validate the results obtained from Python simulation with the results obtained from [21]. To model graphene as a switch explained in the inline methodology in Figure.8 and the plots in Figure.9 are obtained and correspondingly verified with [21]. The aim is to study the change in Band gap of the graphene switch when an external potential U is applied. To apply a potential to the middle region, the onsite_energy_modifier is used to apply potential directly. The corresponding E-k diagram, with and without potential applied is shown below

5 Implementation of Graphene MOSFET

5.1 Using Python for MOSFET Modelling

To study the Graphene MOSFET, unique in its Graphene Channel, we need to study the properties of the Graphene Channel. The modelling of the Graphene Channel is done using Pybinding[11] and the Transportation is calculated using Kwant. Pybinding[16] and Kwant[33] are Python Libraries that allow computation of Tight binding models. The Graphene channel is modelled by defining the nature and structure of Graphene -monolayer, bilayer, zigzag or arm chair. The length and width are defined and leads attached on left and right boundaries. The working of the channel is facilitated by the applying of external potential,

that provides the necessary energy for the motion of charge carriers. The gate-source voltage (V_GS) and drain-source voltage (V_DS) are applied. In Python modelling, they can be applied in 3 different ways. The 1) gate-drain voltage and drain-source voltage is applied in the transport equation, 2) gate-drain voltage is applied to model and drain-source to transport equation and 3) both are applied directly to the model. These different methods allow us trade-off between computation speed and accuracy. Method 3) provides the most reliable results but is computationally expensive. The three methods described above are a natural progression in the work to improve performance.

The MOSFET channel is modelled with Length=10 and 20 nm and width = 2nm. The model is generated using the Pybinding model and then converted to kwant model, using the tokwant() function. The portability to kwant is made available in the Pybinding library. The detailed methodology is discussed in Figure 10. The channel modelled is shown in Figure 11. The structure in Figure.11(a) and 11(b) are obtained by changing the dimensions of the GNR channel of the MOSFET model considered.

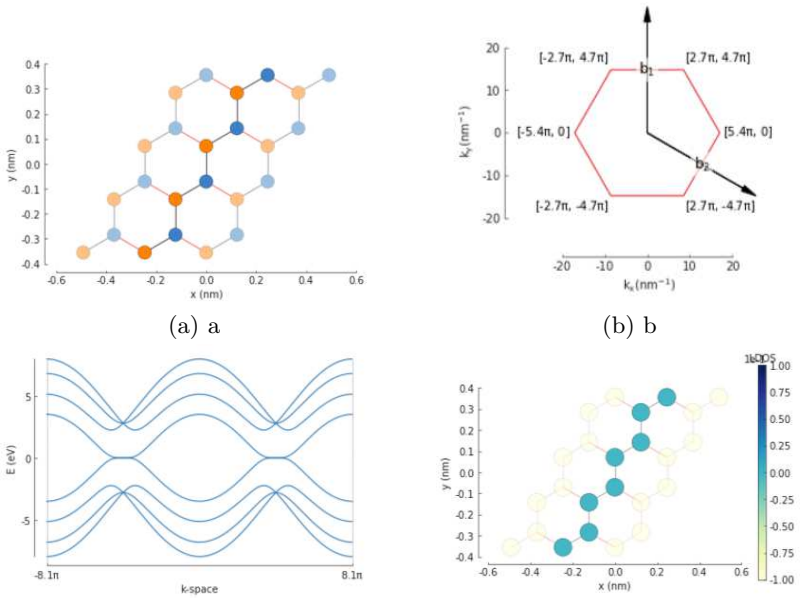
5.2 Using Python for MOSFET Modelling using NEGF

Using the built in function in kwant to solve the Green's equation the conductance v/s transmission graph is plotted as in Figure.12. Figure 12a) shows better conductivity of shorter channel (close to 1) than Figure 12b). And we know that the current transport equation can be plotted using the relation below.

$$I = \frac{-q}{h} \int T(E)\big(f1(E) - f2(E)\big)dE \quad [8] \tag{10}$$

$$f_{1,2} = \frac{1}{1 + exp\frac{E-\mu_{1,2}}{k_B T_{1,2}}} \quad [8] \tag{11}$$

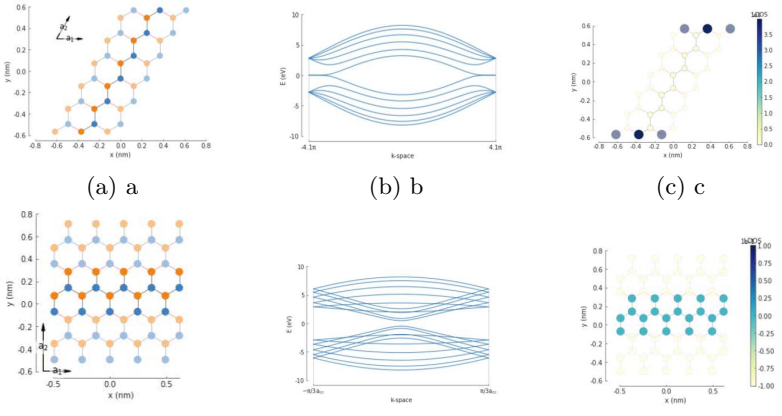
The results are compared with works from [24] and [34]. The results are found to be similar, verifying the performance of Python as a modelling tool for simulating Quantum models.
It is important to note that integration in continuous domain is computationally expensive and all closed form models used in this work use summation. A summation operation is performed to calculate the green's function for the computation of current . The response plotted is for V_DS versus I_D, can be seen in Figure. 13. The channel length and absence of bandgap, the drain current therein is higher and does not show pinch-off [25],[26]. Figure 13 shows the progression in our work in modelling MOSFET in Python. Figure 13a) and b) were modelled using Technique-2 mentioned above and Figure 13c) and d) were modelled using Technique-3.



(a) a (b) b

(c) c (d) d

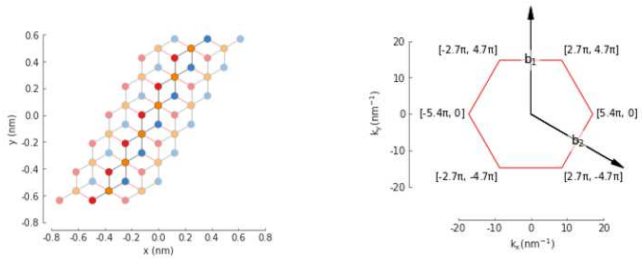
Fig. 5: (a) Monolayer Graphene (b) Brillouin Layer Plot (c) E-k Diagram (d) LDOS Plot



(a) a (b) b (c) c

(d) d (e) e (f) f

Fig. 6: (a) Graphene Nanoribbon zig zag (b) E-k Diagram (c) LDOS Plot (d) Graphene Monolayer Nanoribbon (Arm Chair Edges) (e) E-k Diagram (Arm Chair Edges) (f) LDOS Plot (Arm Chair Edges)



(a) a (b) b

(c) c

Fig. 7: (a) Graphene Bilayer Nanoribbon (b) Brillouin Layer (c) E-k diagram

The steps for deriving the required Graphs for Graphene Switch are as follows-

1) Using Pybinding (Python library for Tight-binding calculations for Graphene) to generate the Channel, using specified Length , and Width and type of graphene (monolayer, bilayer, armchair etc.).

2) To evaluate the properties of a finite object (Allows for the assumption of Translational Symmetry), LEADS need to be attached (attached on the Left and Right Side).

3) On the channel two potentials can be considered to be acting - Gate and Source-Drain. The Gate Voltage allows for conduction through the channel and is applied using Step-4.

4) The potential is defined using the function generator @onsite_modifier - use defined in Pybinding.

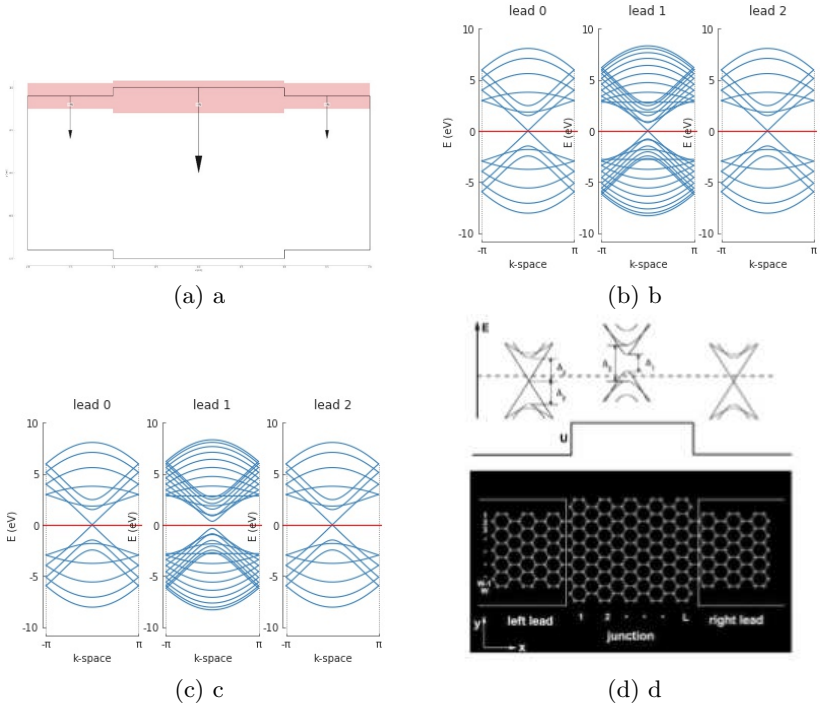
5) The defined Potential allows us to apply electrical fields to the system (refers to the finite Graphene Channel) and can be used to model Gate and Source-Drain voltage (applied to the main model and not leads)

6) The system is compiled and a model is generated (The model comprises of system, leads and any required constants - Pre-built into Pybinding and Positions of atoms in Lattice)

7) The model is passed through a solver (Made-available in Pybinding), that calculates the Hamiltonian Matrix and any other required calculations and stores them in a class object.

8) The class object is passed through the plotter function to plot the three graphs,

Fig. 8: Methodology: The graphene switch structure built in python and the methodology to determine its switching characteristics



(a) a (b) b

(c) c (d) d

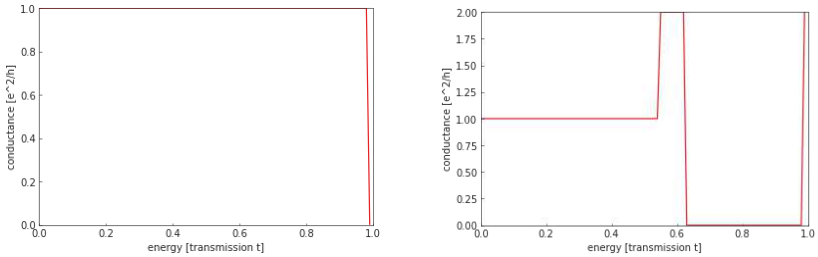
Fig. 9: (a) Switch Structure (b) E-k diagram without potential (c) E-k diagram with potential (d) Results[21]

Steps for Modelling MOSFET
Step-1 Model the Graphene Channel, specifying length and width. Define the potential function using the onsite_modifier function in Pybinding. Apply potential due to Gate and exponential decaying potential due to Drain-Source Bias. The Potential can be modelled with V=V at x=0 at source and V =>0 at x=l.
Step-4 Attach Leads to the Graphene (Across the lengths).
Step-3 Convert the Pybinding model to want using the tokwant() function.
Step-4 Create a smatrix object using the function kwant.greens_function (retarded Green's function) or kwant.smatrix.
Step-5 Use the smatrix.transmission() property to compute the transmission coefficient.
Step-6 Compute the Fermi Functions.
Step-7 Use the formula given in 12 to compute the current (Here we use summation over integration).

Fig. 10: Methodology: Graphene MOSFET I-V characteristics

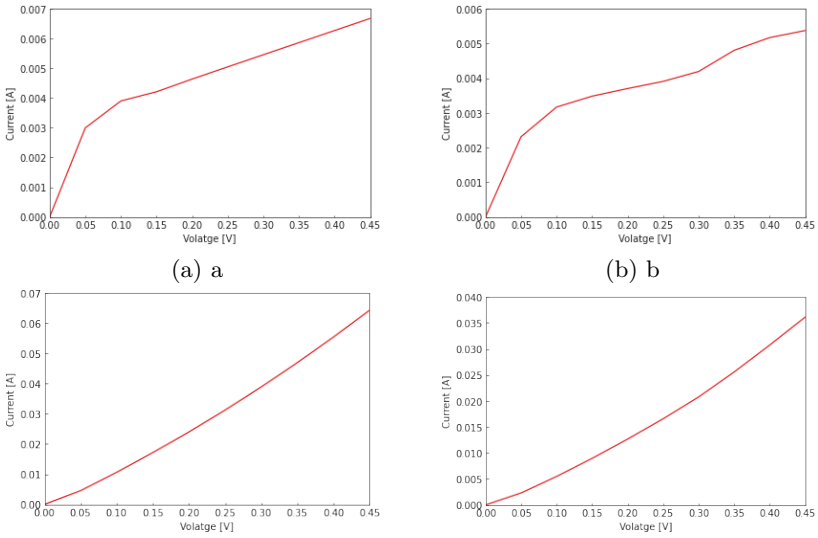
(a) a (b) b

Fig. 11: (a) Graphene Channel-1-L =10 nm, W = 3nm; (b) Graphene Channel-2 (Monolayer), L =20 nm, W= 3 nm



(a) a (b) b

Fig. 12: Conductance v/s Transmission (a) Channel-1 (b) Channel-2 corresponding to structure in Figure.11(a) and (b).



(a) a (b) b

(c) c (d) d

Fig. 13: Transport Characteristic(Technique-2) (a) Channel-1 (b) Channel-2 (Technique-3) (c) Channel-1 (d) Channel-2

6 Conclusions

Graphene based nanoscale devices use bottom-up approaches from molecule to device based on quantum principles to analyze the characteristics of materials and the devices they are used to form. Python as tool has been used here to develop a graphene nanoribbon MOSFET implemented using monolayer graphene channel. The prelude to this is the tight binding approach that have been used to model graphene monolayer, bilayer, graphene nano ribbon using pybinding module tool in python. The E-k plots of different structure of graphene are plotted and verified with the corresponding monolayer, bilayer and nanoribbon structure. A graphene switch is structurally built in python and verified for the performance with a relevant work. The models developed herein also is used to develop GNR MOSFET for different channel lengths of 10nm and 20 nm. These models are built from first principles with 2-D contacts to determine the transport of carriers in the channel and the $I_D - V_DS$ characteristics are plotted. Python modelling is applied in 3 different ways 1) gate-drain voltage is applied to model and drain-source to transport equation, 2) gate-drain voltage is applied to model and drain-source to transport equation to model and 3) both are applied directly to the model. These different methods allow us trade-off between computation speed and accuracy. Method 3) provides the most reliable results but is computationally expensive. The methods described above are a natural progression in the work to improve performance. The future scope is that the graphene based GNR MOSFETs would be extended to implement the applications of logic devices for switching applications by developing P and N MOSFETs. The development of RF circuits using the GNR MOSFET and its application in analog mixed signal is to be explored to determine and analyze delay-power-delay product and performance measures of cut-off frequency.

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7 Declarations

Funding (information that explains whether and by whom the research was supported) - None
Conflicts of interest/Competing interests (include appropriate disclosures) - None
Availability of data and material (data transparency) - Made available after acceptance on GitHub

Code availability (software application or custom code) - Made available after acceptance on GitHub

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