CZECH TECHNICAL UNIVERSITY IN PRAGUE
FACULTY OF ELECTRICAL ENGINEERING

Department of Microelectronics

The Study of the Nanometric Structures

MASTER THESIS

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This thesis was written at the Department of Microelectronics of the Czech Technical University in Prague.

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In Prague on ….. (Bc. Aleksei Barulin)

Dedication: I would like to express gratitude towards my supervisor, Doc. RNDr. Jan Voves, CSc., for the patience, guidance and support throughout my period of study. Next, I would like to thank Ing. Jiří Šmarhák for his help. Last, but not at least, I would like to thank all my family for having faith in me.

Tasks

1. Review the possibilities of preparation and properties of graphene nanoribbons on silicon carbide.
2. Simulate graphene nanoribbons on silicon carbide using suitable tools.
3. Analyze the behavior of the structure, compare with experimental data.
4. Evaluate obtained results.

Original task is applied to printed version of thesis

Title: The Study of the Nanometric Structures

Summary

This project contains simulation of nanoribbons on silicon carbide structures. The first and the second chapter includes brief introduction for not familiar readers. The third chapter describes used calculation methods and models. The fourth chapter shows the simulation process and obtained results. The fifth chapter contains short conclusion.

Key words: nanometric structure, silicon carbide, graphene, graphene nanoribbons

Název: Studium nanometrových struktur

Anotace

V tomto projektu byla provedena simulase grafenových nanopásků na karbidu křemíku. První a druhá kapitola obsahuje základní informace nutné pro orientaci čtenáře, který není s problematikou seznámen. Třetí kapitola popisuje použité výpočetní metody a modely. Čtvrtá kapitola ukazuje simulační proces a dosažené výsledky. Pátá kapitola obsahuje krátké zhodnocení.

Klíčová slova: nanometrová struktura, grafen, karbid křemíku, grafenové nanopásky

Subscripts and superscripts

CMOS	Complementary Metal–Oxide–Semiconductor
BSTO	Barium Strontium Titanate
A-GNR	Armchair Graphene Nanoribbon
Z-GNR	Zigzag Graphene Nanoribbon
GNR	Graphene Nanoribbon
MEG	Multilayer Epitaxial Graphene
e-beam	Electron Beam
UHV	Ultra High Vacuum
EG	Epitaxial Graphene
E_F, E_D	Dirac Point of Graphene
TEM	Transmission Electron Microscopy
HRTEM	High-Resolution Transmission Electron Microscopy
RIE	Reactive Ion Etching Process
XPS	X-Ray Photoelectron Spectroscopy
hν	Energy of Photons
Ψ	Wave Function
$\hat{H}$	Hamiltonian
E	Energy
N	Natural Number
EH	Extended Hückel Method
HMO	Hückel Molecular Orbital Theory
φ_j	Valance Atomic Orbital
h_{eff}	Effective One Electron Hamiltonian
ψ_j	Eigen Function
ϵ_j	The Energy Eigenvalue
DFT	Density Functional Theory
$\rho(\vec{r})$	Probability of Finding Electrons Within Volume
$V_{ext}(\vec{r})$	External potential
E_{tot}	Total Energy
E_{elec}	Electron Energy
E_{nuc}	Nucleon Energy
$\delta_{n,m}$	Kronecker delta
c_m	Constant
$-J$	Probability of Electron Hopping
k	Momentum (wave vector)
FFT2D	Two-Dimensional Fast Fourier Transformation

Contents

1. Introduction

Nanotechnology is becoming more and more attractive nowadays. Electronic devices are becoming smaller and smaller. It is the reason to study inter-atomic interaction and quantum mechanical properties more extensively. Recently, 22 nanometer silicon CMOS technology has already been within this regime, and a lot of resources are being invested to develop a new one to replace. The most popular directions in nanotechnology are hybrid molecular/semiconductor electronics, one-dimensional nanotubes/nanowires and molecular electronic.

Graphene is two-dimensional network of sp^2 hybridized carbon atoms packed into honeycomb lattice. Because of its unique electronic transport properties, graphene has a huge potential for developing molecular devices. These unique properties appear when lower valence and the upper conduction band meet each other at the points, called Dirac points. That is why graphene can be seen as a zero-gap semiconductor or as a zero-overlap semimetal. Around these points energy has linear dispersion. It means that electrons at these states have zero effective mass and are able to gather very high velocity. In the dependence on the substrate, number of graphene layers and other conditions make this spectrum less linear and electron velocity lower. The main goal of this work is to investigate electron transport across one of the most promising structure and to compare it with ideal graphene properties.

The biggest problem, which prevents using graphene nowadays, is difficult synthesis. In the last decades it was synthesized on various substrates, such as gold, copper, nickel, platinum and ruthenium. However, the most convenient way to obtain a single layer or a few layers of graphene is to use carbon containing electrically insulating crystals, such as diamond and silicon carbide. Silicon carbide is a natural candidate for the graphene technology at this moment, because it is a useful semiconductor and, by post growth thermal treatment, epitaxial films can be produced that exhibit all the transport properties of ideal, two-dimensional graphene. Both polar surfaces (Si- and C- terminated) can be also used, but their potential depends on the properties of the synthesized graphene.

1.1 Graphene Based Devices

Previously, great hope was pinned on using graphene in high frequency transistors, in digital logic and analogue circuits. It is foreseen that silicon-based transistors in digital logic will eventually have to be replaced to enable the continuation of performance improvements following Moore's law. Therefore, there is an intensive search for the replacement materials. While high frequency operation up to 300 GHz has been shown for graphene transistors, and predictions estimate that it could be pushed to the THz range, the lack of a band gap makes it difficult to achieve a low leakage current in digital logics and a large power gain in analogue applications. There are several ways to open a band gap in graphene, but so far it is not possible to achieve a sizeable band gap with high charge carrier mobility. It is unclear whether it is a fundamental limitation and whether we will ever see a carbon-based processor.

Not all electronics require extremely high carrier mobility. Ink-jet printed electronics are low-cost devices for a variety of applications where a modest electronic performance is acceptable. Traditionally, the charge carrier mobility for this technology is less than 1 $cm^2V^{-1}s^{-1}$. Using graphene-based inks can improve the mobility to ~ 95 $cm^2V^{-1}s^{-1}$, an improvement of two orders of magnitude. Graphene-based inks are the first commercially available products based on graphene.

Graphene can also find its place within several energy applications. It can be used as an electrode in batteries, for fuel- and other electrochemical cells, and in ultracapacitors.

Such a comprehensive list of potential applications has initiated a rush for immaterial property connected with graphene.

Graphene is planar technology, which is easy to implement in most fabrication processes. In this case, it can be compared to diamond-like carbon, which is planar carbon (mostly sp^3-hybridized) and is used in great volumes in many applications.

There exist many different types of graphene depending on the method of fabrication and its integration. These types are essentially different materials with different properties and applications. Therefore, it is more correct to talk about a graphene material family, rather than the single material. In this case, they do not all share the same strengths and weaknesses, making it more likely that at least some could succeed.

For the one atom thin semimetal graphene the capacitively induced surface charge concentration is in the order of 10^{13} cm^{-2} by a gate electrode is enough to drastically change the graphene properties. Depending on the sign of the applied gate voltage, the carrier concentration can be tuned from holes to electrons, showing the bipolar field effect. Because of thermal fluctuations, nonuniformities in the graphene, impurities, electrical charges in the vicinity of graphene, etc. there is always a minimum residual charge carrier concentration in any graphene device despite tuning by gate. The Dirac point, where the resistance reaches the maximum, is close to the zero gate voltage where the minimum carrier density is. In practical devices the Dirac point is often shifted from zero voltage due to charged impurities in the vicinity of graphene.

Because of the strong field effect, graphene can be used in ferroelectrics. In combination with a ferroelectric substrate, graphene can be used as a read-out of ferroelectric state. Such devices were first produced by applying a ferroelectric polymer on the top of standard graphene devices on SiO_2 and on flexible transparent substrates. Graphene on ferroelectric BSTO substrates exhibits a strong unusual resistance hysteresis, which can be utilized as a simple read-out in a graphene-ferroelectric hybrid memory device. The shape of hysteresis can be related to many phenomena including the charge trapping in the oxide or on the surface of graphene, or to the dynamics of surface bound water molecules. [1]

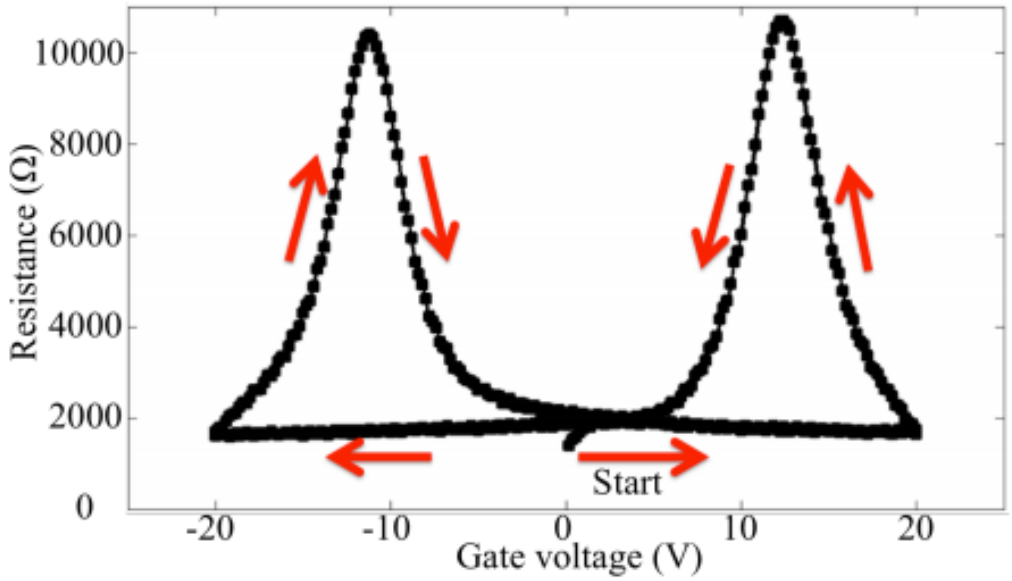

Figure 1.1.1: Resistance as a function of gate voltage for graphene on the top of ferroelectric BSTO at 4 K. Two distinct resistance maxima are observed depending on the sweep direction of the gate voltage. The two peaks are symmetric and well separated. The hysteresis is opposite of that one would expect from a pure switching of the ferroelectric state. [1]

2. Graphene Electronics – State of Art

2.1 Graphene Structure

Before starting the complex analysis of epitaxial graphene, we need to look at the ideal infinite, electronically isolated two dimensional hexagonal sheet of carbon atoms, as shown on Figure 2.1.1 a. The standard in-plane unit cell vectors are $|a_G| = |b_G| = 2.4589$ Å. The unit cell contains 2 carbon atoms at (0,0) and $(a_G/3, 2b_G/3)$. It gives a carbon areal density of 3.820 atoms $Å^{-2}$. Graphene bonds are hybridized into a sp^2 configuration. These bonds are extremely strong and form the rigid backbone of the hexagonal structure.[2]

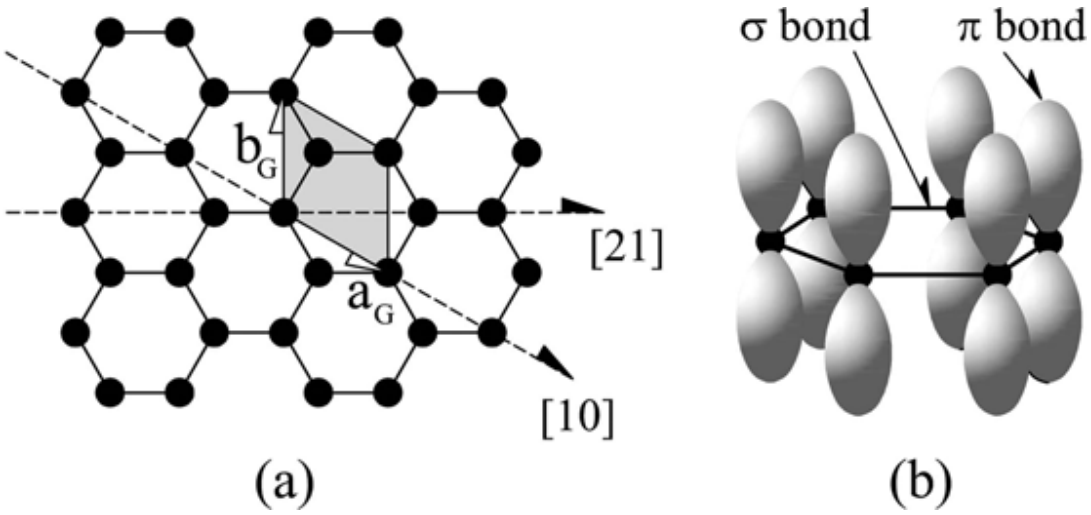

Figure 2.1.1: Graphene structure
a) Graphene hexagonal structure of identical carbon atoms. The unit cell (shaded) containing two carbon atoms is shown along with standard unit cell vectors $\mathbf{a}_G$ and $\mathbf{b}_G$. The 'armchair' edge and the 'zig-zag' directions are shown.
b) Schematic of the in-plane σ bonds and the π orbitals perpendicular to the plane of the sheets.[2]

Now let us project this lattice into reciprocal space and Brillouin zone. Points K at the corners of the zone have the particular importance for the physics. (Figure 2.1.2)

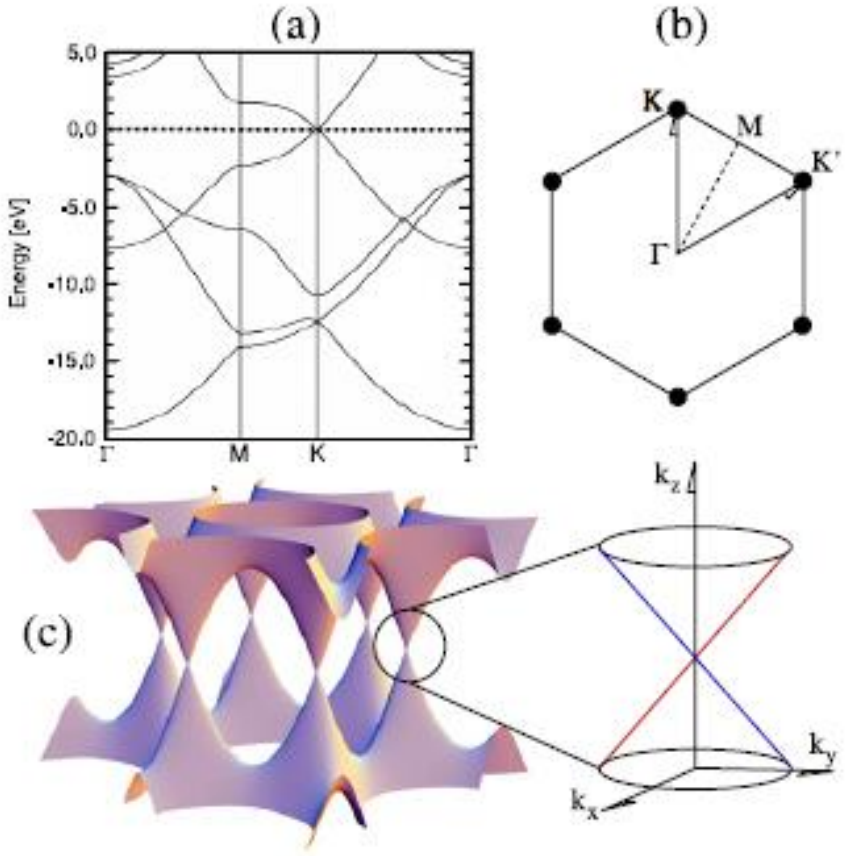

Figure 2.1.2:
a) An *ab initio* band structure calculation of graphene.
b) A schematic of the Fermi surface of graphene consisting of points intersecting the Dirac cone.
c) The two dimensional tight binding energy surface of graphene. [2]

These important points are named Dirac points and related to a particular feature of the electronic band-structure of graphene and they appear due to the intersecting bands of two equivalent carbon sublattices A and B (Figure 2.1.1). The energy dispersion at these points is linear. The linear dispersion also leads to another important property. Electrons and holes cannot be described by independent Schrödinger equations. Instead, the electrons and holes are represented as quasi-particles connected in the way described by the Dirac equation. Electrons and holes are described by a pseudospin that is parallel to the electron momentum, but opposite to the hole momentum. It means, that electrons cannot hop from K to K' since the pseudospin is not conserved. This rule gives rise to the ballistic transport observed in graphene. [2]

2.2 Graphene Nanoribbons

When infinite graphene crystal becomes finite, surface and boundaries appear, forming atoms at the edges without the third neighbor carbon atom. If the size is in the order of nanometers, graphitic nanostructure exhibits different properties from those which were observed in an infinite layer. Among these graphitic nanostructures are nanoribbons and nanoclusters. In analogy with the 2D counterpart, it can have graphene-, bilayer-, few-layer- and graphitic-nanoribbons or nanoclusters. It is noteworthy that fullerenes, graphitic nanotubes and related structures, such as toroid and carbon helixes, can be treated as separated systems since bending needs to be considered and curvature effects play an important role. In general, a graphitic (graphite or graphene) nanoribbon could be defined as a one-dimensional sp^2-hybridized carbon crystal with boundaries that expose non-three coordinated carbon atoms. It possesses a large aspect ratio.

Graphene nanoribbons have borders which can exhibit edge states and different electronic, chemical and magnetic properties depending on the size and type of the border. The most studied chiral edge configurations, 0° (armchair) and 30° (zigzag), lead to armchair and zigzag nanoribbons (A-GNRs, Z-GNRs).

Z-GNRs exhibit edge states, which are not presented in the armchair case. These edge states are presented as a flat band around the Fermi level, but extended along the ribbon's edge. It leads to a metallic nanoribbon if the width is large enough (e.g. > 10 nm). Such flat band leads to a high density of states located at the edges, indicating that they are very reactive sites. Furthermore, Z-GNRs exhibit magnetic properties that are relevant for spintronics. [3]

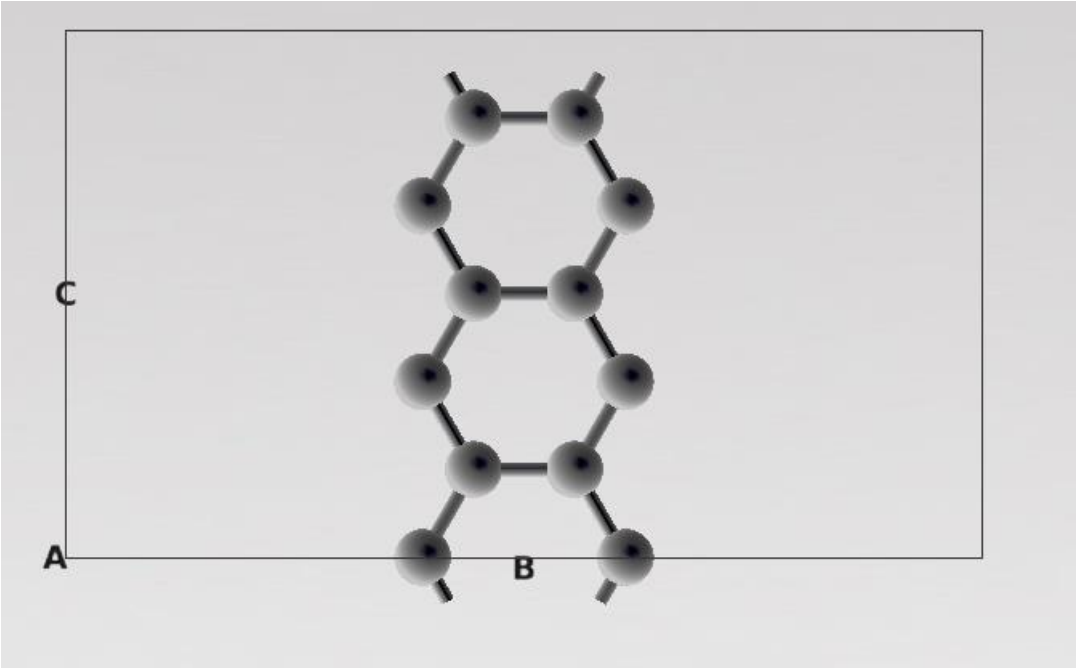

Figure 2.2.1: Graphene nanoribbon with zigzag edge and 4 atoms wide

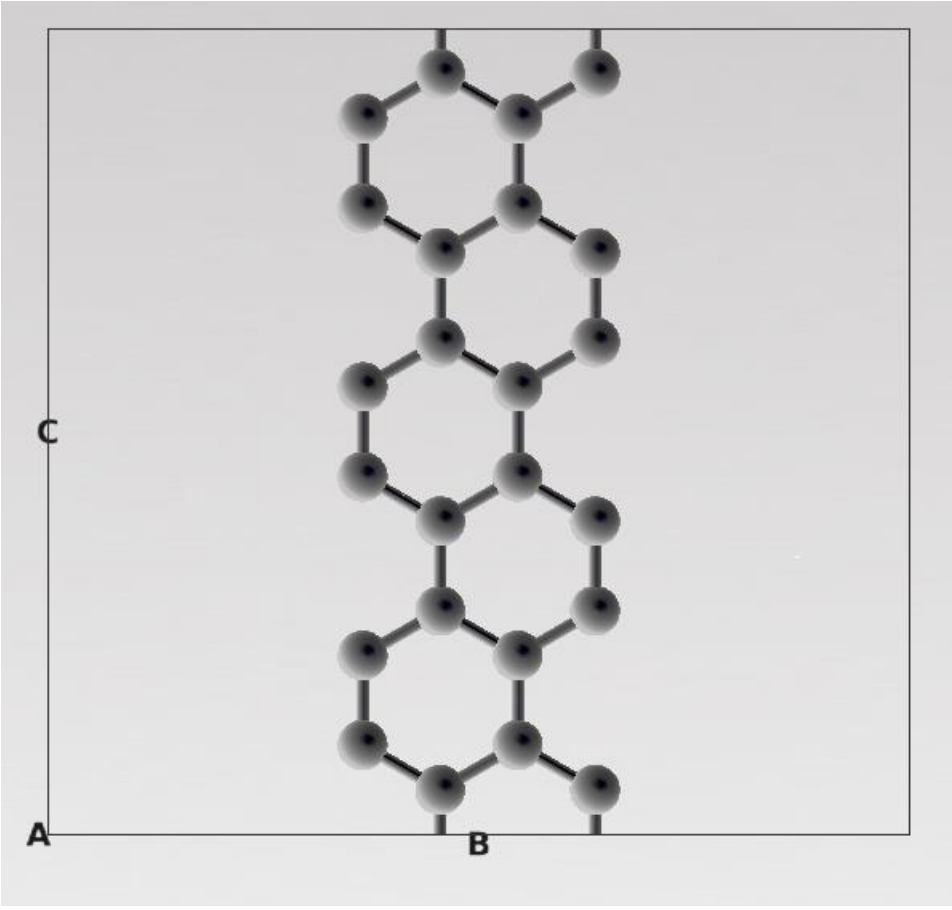

Figure 2.2.2: Graphene nanoribbon with armchair edge and 4 atoms wide

The properties of A-GNRs have a dependence on the width. In order to produce materials with band gaps E_g ~ 0.7 eV the width of ribbon must be between 2 and 3 nm. To increase the bang gap the ribbon widths must be reduced to 1-2 nm, and the width increasing make the band gap tend to the zero value of 2D graphene.

The unusual electronic and transport properties of GNRs indicate that these carbon nanomaterials could be excellent new building blocks in the future carbon based nanoelectronics, thus opening alternatives to the current silicon-based electronics, through the using of new variable states (e.g. quantum states, spin, etc.). [3]

2.3 Silicon Carbide Properties

Silicon carbide is composed by tetrahedral of carbon and silicon atoms with strong bonds in the crystal lattice. It produces a very hard and strong material. In the air conditions, SiC forms a protective silicon oxide coating at 1200°C and is able to be used up to 1600°C. The high thermal conductivity coupled with low thermal expansion and high strength give to these materials exceptional thermal shock resistant qualities. Silicon carbide ceramics with a little or no grain boundary impurities maintains the strength against very high temperatures, approaching 1600°C with no strength loss. Chemical purity, resistance to chemical attack, and strength retention at high temperatures has made this material very popular as wafer tray supports and paddles in semiconductor furnaces. In Table 1 (see Appendix A) all main properties of SiC are presented. Silicon carbide has huge bad gap (at room temperature). Which allows using this material as an insulator in graphene based devices. [4]

2.4 Epitaxial Graphene

The main problem of graphene nanotubes and nanoribbons are difficulties in the control of the position, radius, chirality and length very difficult. It is more desirable to prepare the graphene directly on an insulating substrate, then pattern the graphene in the areas where it is required, with a process flow similar to one used for silicon-on-insulator devices. A graphene grown on insulator allows integration of large scale circuits, not just individual devices. A process of generating graphene on insulator, or

more specifically multilayer epitaxial graphene (MEG) on SiC (MEG/SiC), has been developed through the high temperature sublimation of silicon from SiC. [5]

Growing thick graphite samples on SiC has been a well-known process for many years until the thickness was decreased to a few layers, and a full characterization of the high quality graphene sample carried out. The growth of epitaxial graphene on SiC is based on thermal decomposition of the SiC substrate. E-beam heating as well as resistive heating is used, but no difference seems to arise from the different heating methods. In order to avoid contamination the heating is usually performed in ultra-high vacuum (UHV) environment or sometimes with Ar gas. Similar results were observed for the high and/or low base pressure growth, but so far no comparative study about the influence of the background pressure in the vacuum chamber was conducted. From the molar densities one can calculate that approximately three bilayers of SiC are necessary to set free enough carbon atoms for the formation of one graphene layer. The growth of the graphene can take place on the (0001) (silicon-terminated) or $(000\bar{1})$ (carbon-terminated) faces of 4H-SiC and 6H-SiC wafers. The main difference lies in the sample thickness that one can achieve. In the case of the silicon face, the growth is slow and terminates after relatively short time at high temperatures leading to the rise of very thin samples, down to a monolayer. On the contrary, in the case of the carbon face, the growth does not self-terminate leading to the rise of the relatively thick samples (approximately 5 up to 100 layers) with larger orientation and turbostatic disorder. [6]

One of the biggest hurdles for graphene to be useful as an electronic material is its lack of an energy gap in the electronic spectra. For example, it prevents the graphene from using in making transistors. The interaction between the graphene layer and the substrate will break the A and B sublattice symmetry, which opens a band gap. When graphene is grown on the SiC substrate, a gap of $\approx 0.26\,\mathrm{eV}$ is produced. This gap decreases while the sample thickness increases and eventually approaches zero when the number of layers exceeds four. [5]

2.5 Graphene-Silicon Carbide Interface

The Graphene/SiC interface model is very complicated. Because of the relations between graphene and SiC lattice constants, there is a large number of possible orientations of graphene. One structure of particular relevance is the ($6\sqrt{3}$ x $6\sqrt{3}$)R30 structure. The ball model of this appropriate graphene structure is shown in

Figure 2.5.1. Note the high symmetry points of the graphene lattice relative to the SiC (shaded hexagons). There are points where either the carbon atom in the graphene layer sits directly above an atom in the SiC layer below, or a SiC atom lies directly below the center of a graphene hexagon. We can define a quasi-unit-cell that is defined by these high symmetry points. For the appropriate ($6\sqrt{3}$ x $6\sqrt{3}$)R30 structure shown in Figure 2.5.1 the quasi-cell would be a (6 x 6) SiC unit cell. [7] The primary cell of this structure is long and it takes long time to proceed one calculation. So this cell is usually artificially decreased. As a result we get simple model of graphene sitting above a relaxed bulk bilayer. Models like this cannot accurately describe the interface layer, but can predict a number of important results. Firstly, the relaxed distance between the last substrate atom and the first graphene layer is larger on the Si-face (about 2.0 Å) than on C-face. Secondly, the evolution of the band structure with the number of graphene layers can be predicted. The first graphene layer, which is more tightly bounded to the substrate, has a significant distortion of the π-bonds that gives the growth to a gap in the band structure. This first graphene layer shows no evidence of a graphitic electronic nature. The second graphene layer has the linear dispersion at the K-point characteristic of an isolated graphene sheet. Thus, in these calculations, the first graphene layer on both substrates acts as a 'buffer' layer electrically isolating the second graphene layer from the substrate. The third graphene layer shows splitting of the hole and electron states at the K-point stacked graphene bilayer.

It is important to realize that, as the graphene forms, the surface of the sample will recede when Si atoms are leaving. The carbon content in a single graphene monolayer is very close to three SiC bilayers (36.5 atoms/nm^2). The latter constitutes 0.75 nm of the height in its SiC form, whereas the graphene monolayers are spaced by about 0.34 nm from each other and have similar spacing to the SiC (for the C-face) or the $6\sqrt{3}$ layer (for the Si-face). Thus, for each additional monolayer of graphene, the top surface must recede by about 0.4 nm. So, if graphene thickness is different across the sample, thickness of substrate is different as well. Also, graphene thickness is measured in number of graphene layers, which is discrete number. Assume sample with 1, 2, 3 and 4 monolayers graphene thickness on it. The morphology of the surface of such sample changes: now is covered by step edges. With the flat regions of the surface, steps form irregularly-shaped μm-sized regions, which are separated from their neighboring terraces by step bunches.

By having a very wide range of graphene domain thicknesses, the C-face is much different to Si-face. The large range in graphene thicknesses for the C-face, essentially a 3D growth phenomenon, is expected to have significant deleterious effect on electrical behavior.

To archive a narrower distribution of the thickness-domains on the C-face, while maintaining a relatively thin film, higher temperature in an argon environment is needed. This method was developed to reduce the sublimation rate of the Si. The method works very well on the Si-face, where annealing in 1 atm of Ar at 1600°C is used to produce large domains of single thickness (1 monolayer) graphene. For C-face graphene with the same conditions is possible to get 2 results: there is no graphene layer at all or there are very thick graphene films.

In vacuum, it appears that the initial graphene formation on the C-face is not so different than on the Si-face. In both cases the initial lateral extent of constant-thickness (1 or 2 monolayers) domains of the graphene is < 100 nm. With subsequent annealing the C-face graphene morphology coarsens, forming large areas with 2 monolayers coverage, as well as small areas with 3 monolayers coverage. This process continues until the several-μm-sized domains of graphene become thicker. However, the lateral extent of the domains does not further increase for the C-face, even for thickness up to 8 monolayers, and the range of thicknesses on the C-face is about 5 monolayers whereas it is limited with a single monolayer for the Si-face.

If we compare the Si-face and C-face graphene morphologies for a fixed film thickness, we can find that they are very different. But if we compare them at fixed temperatures, the differences become understandable. At ≈1320°C. The films thickness on the C-face is much greater than for the Si-face (16 vs. 2 ML), but both films display the characteristic ridges associated with strain relaxation. Both surfaces display comparable amounts of step bunching. The reason for choosing the thicker film on the C-face is that the $(\mathbf{000\bar{1}})$ surface and $(\mathbf{000\bar{1}})$/graphene interface have higher energies (are more unstable), respectively, than the (0001) surface and (0001)/graphene interface. Additionally, more defects in the C-face films such as the discontinuities and rotational domain boundaries can lead to easier Si diffusion through the graphene, which will also provoke thicker growth.

When graphene is based on the Si-face in 1 atm of argon, the tendency to grow in a layer-by-layer manner becomes even more pronounced. In that case, it is quite easy to produce a single monolayer extending over 10's or 100's of μm on the surface. But for

the C-face in argon, only 3D formation of islands is presented in initial stage of graphene formation, with these islands growing relatively thick (>5 monolayers), before the complete graphene coverage is achieved.

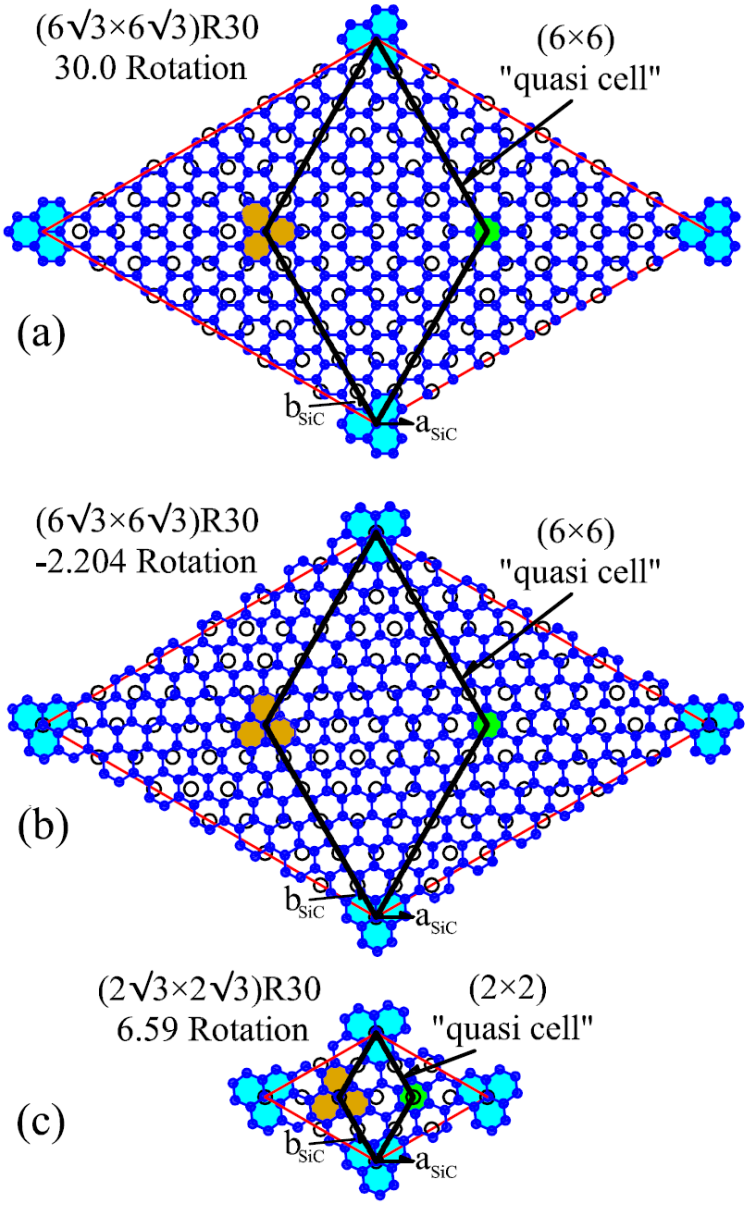

Figure 2.5.1:
a) and **b)** are two graphene–SiC *(*6√3 × 6√3*)*R30 unit cells, one with graphene rotated 30◦ and the other with graphene rotated −2.204◦ relative to the SiC unit cell (red/light grey line). Open circles are atoms in the SiC. Filled circles are C atoms in the graphene layer. The shaded area shows high symmetry points between the graphene lattice and the SiC lattice. A *(*6 × 6*)* unit cell connecting the high symmetry points is also shown.
c) A*(*2√3 × 2√3*)*R30 cell with graphene rotated 6.59 is also shown with its quasi-*(*2 × 2*)* cell. [7]

2.6 Graphene on Si-face SiC

As indicated above, the electronic properties of EG on SiC are layer dependent. An important fact is that the buffer layer has an energy gap at E_F, so transport experiments and valence spectroscopies measure the effect of the graphene layers. The experimental *E(k)* is linear, with a characteristic band velocity consistent with the band structure of an ideal monolayer. Close examination of the spectrum reveals a small shift of the energy bands above the Dirac (charge neutrality) point E_D relative to the bands below E_D. It was ascribed to many-body interactions or to the creation of a small band gap. The parabolic energy bands of layer 2 graphene are apparent, as is the lower energy split-off band. These observations are predicted for bilayer graphene. The small energy gap centered around -350 meV is the result of the interface electric field; it can be driven to zero by balancing the interface field with an electric field contributed by surface adsorbates. Carrier density is also a layer dependent quantity in EG. The charge neutrality point shifts with respect to the Fermi level (zero tunnel bias) for successive EG layers on SiC(0001). [12]

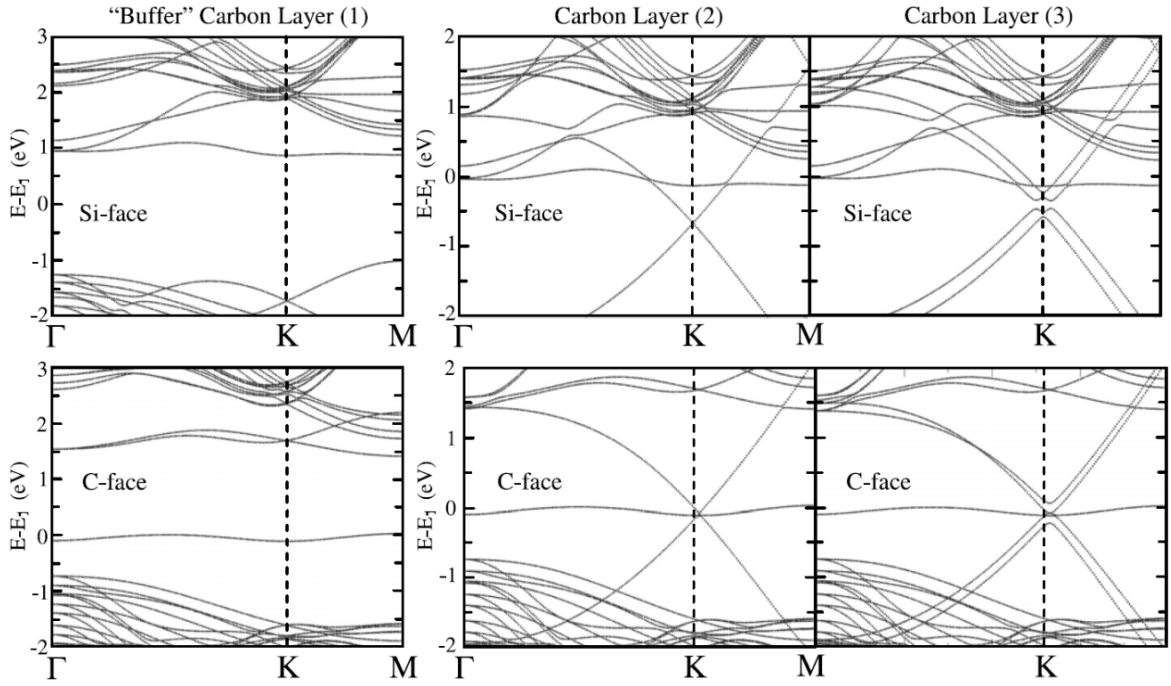

Figure 2.6.1: Band structure for different numbers of graphene layers on both the Si-face and the C-face of SiC. [12]

Also, graphene films have a fixed rotational orientation with respect to the SiC substrate on the Si-face (distinct spots rotated by 30° relative to the SiC spots).

2.7 Spin Filtering Properties of Graphene

The ability to single out one graphene plane through exfoliation process or by mean of epitaxial growth, opened novel opportunities to explore low dimensional transport properties, especially spin transport properties. Usually, graphene nanoribbon with the nanometer sized width has two kinds of edges, the zigzag edges and the armchair edges. Their electronic transport properties greatly depend on their boundary conditions, their edges. Armchair edges can be either metallic or semi-conducting while zigzag shaped edges are always metallic.

The passivated zigzag graphene nanoribbons composed of 2 or 4 atoms wide basis produce strong spin-dependent behavior resulting in a large spin polarization effect. Relying on experiment introduced in [8], for 2 wide zigzag graphene nanoribbon spin up electron eigenstates are strictly placed on the edge of the ribbon, the spin down electron eigenstates are placed inside the ribbon. There are free energy levels only able to transport electrons with spin down in the vicinity of the Fermi level. For energies greater than zero there is greater transmission for spin up electrons at positive energy levels and spin down at negative. For 4 atoms wide nanoribbons the behavior is almost the same, the only difference is that the spin down electrons transmission is almost fully restrained for some small negative energy levels and the transmission spectrum itself is more symmetrical than in the 2 wide variant.

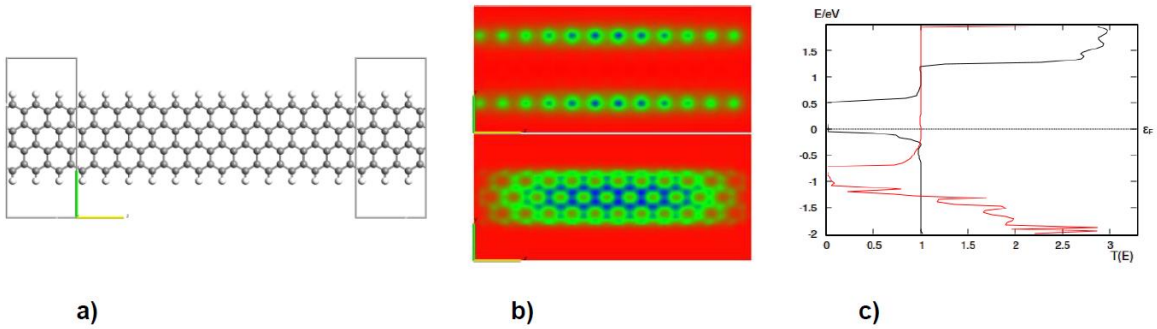

Figure 2.7.1:
a) The simulated system.
b) Eigenstates for the quantum number 0, for the spin UP electrons at the top and for the spin DOWN at the bottom. The color range covers the eigenstate values from their minimum (blue) to maximum (red).
c) Transmission spectrum for the spin UP (black) and DOWN (red). [8]

The strict distribution of electrons with spin up and down allow us to make an assumption that any impurities and distortion in nanostructure will suppress one type of spin and pass the other one.

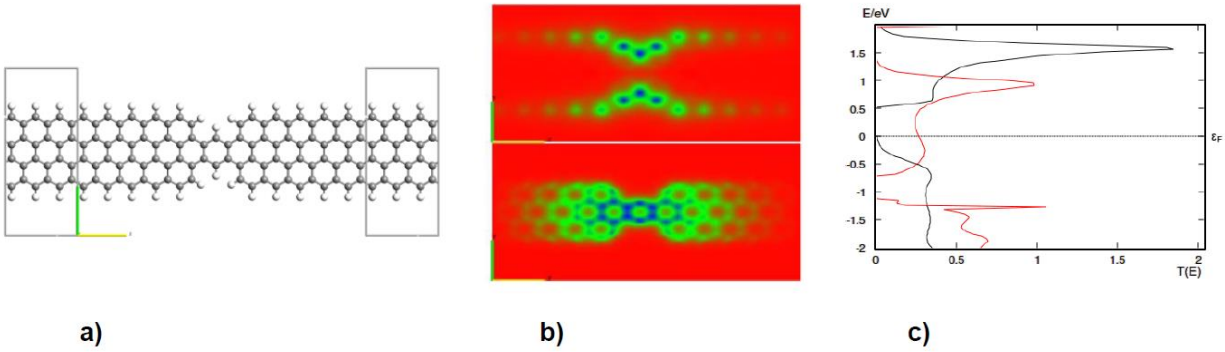

Figure 2.7.2:
a) The simulated system.
b) Eigenstates for the quantum number 0, for the spin UP electrons at the top and for the spin DOWN at the bottom. The color range covers the eigenstate values from their minimum (blue) to maximum (red).
c) Transmission spectrum for the spin UP (black) and DOWN (red). [8]

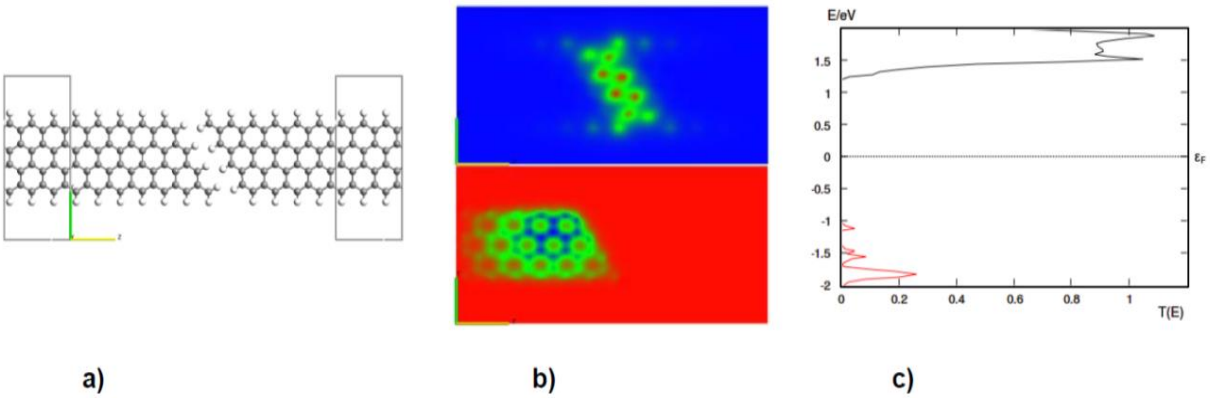

Figure 2.7.3
a) The simulated system.
b) Eigenstates for the quantum number 0, for the spin UP electrons at the top and for the spin DOWN at the bottom. The color range covers the eigenstate values from their minimum (blue) to maximum (red).
c) Transmission spectrum for the spin UP (black) and DOWN (red). [8]

2.8 Step Shape of Silicon Carbide

Existing nanoribbon fabrication methods are slow and often produce disordered edges that compromise electronic properties. The method of the graphene nanoribbon growing, which allows to avoid post-processing damage and can specify position of nanoribbons on the substrate, is introduced in [9]. The morphology of epitaxial graphene on SiC is highly influenced by the underlying SiC structure. Steps on substrate can lead to the problem with proper graphene growing without junk effects, but for few-nm steps the graphene lattice is continuous.

It is well known fact, that SiC{0001} surfaces exhibit step bunching. Steps which are perpendicular to the directions $\langle 1\bar{1}00 \rangle$ are strongly favored on (0001). It is perhaps expected that epitaxial graphene growth should proceed first on nanofacets. Fabrication of the graphene, based electronic device, can be useful (see fig. 2.8.1 and fig. 2.8.2).

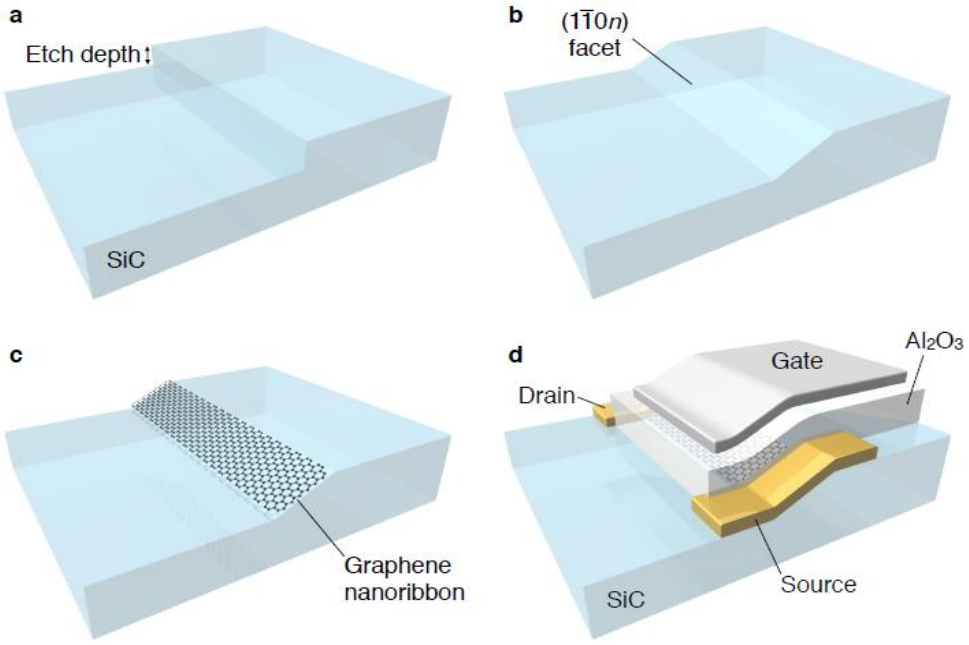

Figure 2.8.1: Process for tailoring of the SiC crystal for selective graphene growth and device fabrication.
a) nm-scale step is etched into SiC crystal by fluorine-based RIE.
b) Crystal is heated to 1200-1300°C (at low vacuum), inducing step ow and relaxation to the (1$\bar{1}$0n) facet.
c) Upon further heating to ~1450°C, self-organized graphene nanoribbon forms on the facet.
d) Complete device with source and drain contacts, graphene nanoribbon channel, Al_2O_3 gate dielectric, and metal top gate, as pictured in Fig. 5b. [9]

High temperature annealing causes vertically etched steps (on the order of 10 nm deep) to produce (1-10) facets with a normal that has an angle of 23° with respect to the {0001} direction.

Cross sectional, high resolution transmission electron microscopy of the graphene on steps on SiC has shown that the graphene terminates perpendicular to the silicon carbide surface both on the bottom of the step or on the steps themselves. This effect was observed using scanning tunneling microscopy on small graphene islands on (0001) SiC. Moreover, these atomic resolution studies further show that the graphene edges are along the zigzag direction, indication that the graphene sidewall ribbons are zigzag ribbons. This is very important when the edge structure determines the electronic properties of the ribbons. In particular, zigzag ribbons are always metallic.

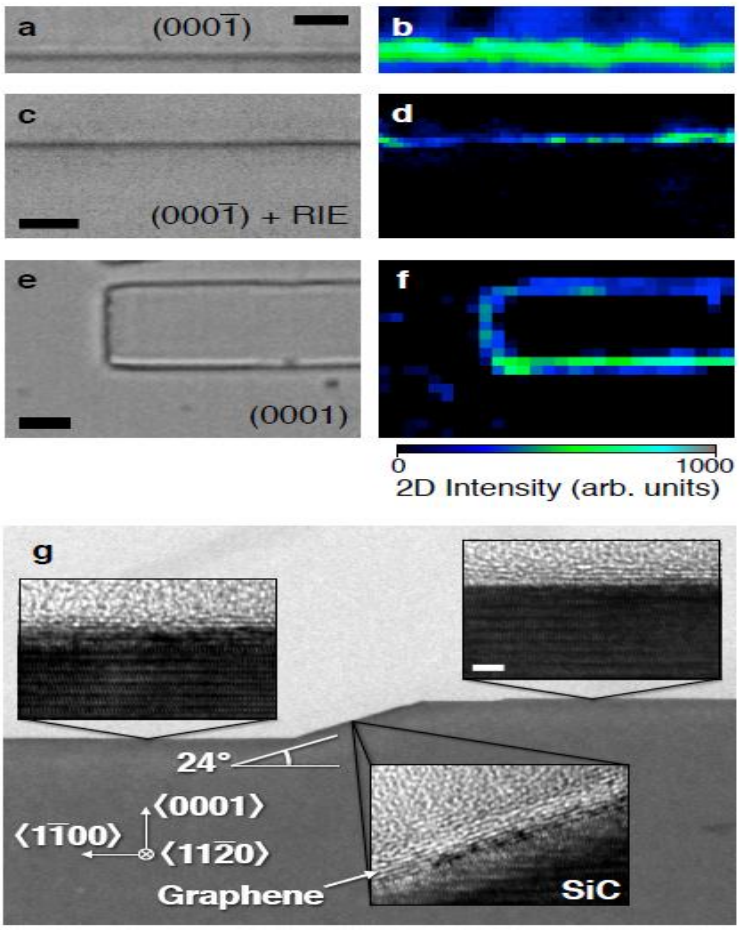

Figure 2.8.2: Raman and TEM observations of graphene grown selectively on SiC nanofacet $(1\bar{1}0n)$ with n ≈ 8. [9]
a) Optical micrograph of pre-patterned 100 nm step on the SiC$(000\bar{1})$ face following graphene growth. Scale bars in (a, c, e) are 2 μm.
b) Raman map (~1μm lat. res., 0.25 μm grid) of the 2D peak intensity at this location indicates preferential graphene growth on the $(1\bar{1}0n)$ facet.
(c - d) Optical micrograph and Raman map of step on SiC $(000\bar{1})$ following exposure to directional O_2 RIE.
(e - f) Optical micrograph and Raman map demonstrating fully selective growth on SiC (0001) without post-treatment.
g) HRTEM cross-sectional images of a similar step on (0001) confirm preferential growth on the $(1\bar{1}0n)$ facet. Scale bar is 2 nm, and applies to all insets.

The zigzag nature of the graphene edges is further confirmed in electron diffraction images of carbon nanotubes grown on SiC, which are always the zigzag variety. It indicates that they terminate with a zigzag edge on the silicon carbide surface. Very important observation with profound implications for graphene nano-electronics is that the sidewall graphene ribbons have zigzag edges in SiC. For one thing, it implies that the edges are passivated and well defined, that they are not subject of the chemical reactivity and the structural disorder of lithographically patterned graphene structures. [10]

In [10] are introduced experimental results of produced graphene structures by using standard lithography methods of producing an etch mask on the surface. Then, the masked surface was subjected to a plasma etch to etch the desired pattern to a predetermined depth into the surface. Then at temperature of about 1550°C, in about 10 minutes, the monolayer of graphene has been grown over the step. It presents an important step towards the realization of high mobility quasi one dimensional graphene structures that do not suffer from the strong localization effects observed in conventionally patterned graphene structures.

In [11] the possibility of graphene production is also shown and resistivity of graphene was measured. According to experimental data, graphene with length about 1.6 μm and width about 39 nm has resistivity 26.1 kΩ.

2.9 Hydrogenation of Graphene

Hydrogen can saturate the silicon dangling bonds without a real decoupling of the interface. In these conditions the charge transfer to the graphene layer is reduced and, as a consequence, the carrier concentration decreases and the carrier mobility increases by about a factor of 2 to 5. The treatment is robust against nanofabrication and thermal cycling, from room temperature down to cryogenic temperature. [12]

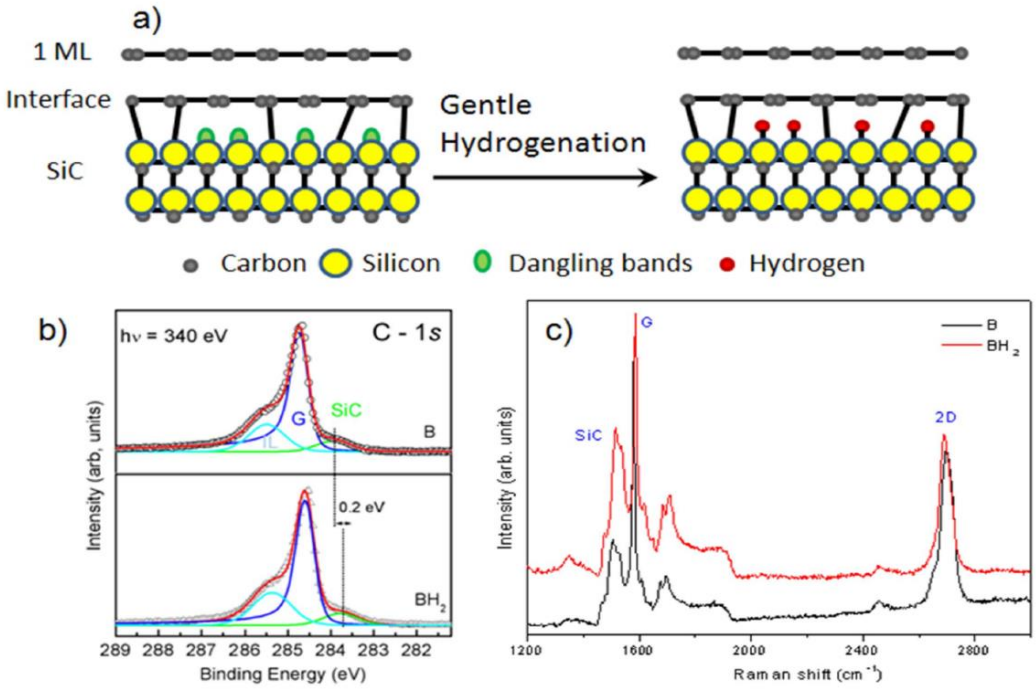

Figure 2.9.1: Structural Properties of Epitaxial single-layer graphene after hydrogenation. [12]
a) Schematic representation of hydrogenation process: after hydrogen exposure the Si dangling bonds between SiC and interface are saturated by hydrogen.
b) C 1s XPS spectra for epitaxial graphene after hydrogenation at 820°C at hν = 340 eV. XPS measurements were performed at φ = 45° emergency angle with respect to the sample normal. This spectrum shows the presence of the interface layer after hydrogenation.
c) Typical Raman spectra of the graphene sample after hydrogenation. Contributions at the G and 2D band are observed, together with a very low signal at the defect band D.

3. Models and Methods

3.1 Extended Hückel Method

The main goal of the most approaches in solid state physics is the solution of the time-independent, non-relativistic Schrödinger equation

$$\hat{\mathrm{H}}\Psi_i\left(\vec{x}_1, \vec{x}_2 \ldots \vec{x}_n, \vec{R}_1, \vec{R}_2 \ldots \vec{R}_m\right) = E_i\Psi_i(\vec{x}_1, \vec{x}_2 \ldots \vec{x}_n, \vec{R}_1, \vec{R}_2 \ldots \vec{R}_m) \quad (1)$$

$\hat{\mathrm{H}}$ is a Hamiltonian of the system consisting of *n* electrons and *m* nuclie.

When the system is in the state Ψ, the expectation value of energy is given by

$$E[\Psi] = \frac{\langle\Psi|\hat{\mathrm{H}}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \quad (2)$$

Full minimization of the function $E[\Psi]$ with respect to all allowed N-electrons wave functions will give us the true ground state $[\Psi_0]$ and energy $E[\Psi_0]$.

Extended Hückel Method is used for an electronic structure calculation. To solve this problem analytically many integrals must be evaluated followed by a self-consistent process for assessing the electron-electron interaction and then electron correlation effect must be taken into account. Semi-empirical methods do not proceed analytically in addressing these issues, but rather use experimental data to facilitate the process. One of the first developed semi-empirical methods was Hückel Molecular Orbital Theory (HMO). HMO was developed to describe molecules containing conjugated double bonds. HMO considered only electrons in pi orbitals and ignored all other electrons in a molecule. It was successful theory, because it could address a number of issues associated with a large group of molecules at the time when calculations were done on mechanical calculators.

The Extended Hückel Molecular Orbital Method (EH) grew out of the need to consider all valence electrons in a molecular orbital calculation. By considering all valence electrons, chemists could determine molecular structure, compute energy barriers for rotation about bonds, and even determine energies and structures of transition states for reactions. The computed energies could be used to choose between proposed transitions states to clarify reaction mechanisms.

In the EH method, only the n valence electrons are considered. The total valence electron wave function is described as a product of the one-electron wave functions.

$$\Psi_{\text{valence}} = \psi_1(1)\psi_2(2)\psi_3(3) \dots \psi_j(n) \tag{3}$$

where *n* is the number of electrons and *j* identifies the molecular orbital. Each molecular orbital is written as a linear combination of atomic orbitals (LCAO).

$$\psi_j = \sum_{r=1}^{N} c_{jr}\varphi_j = 1, 2, \dots N \tag{4}$$

where now the φ_j are the valance of atomic orbitals chosen to include the 2s, 2px, 2py and 2pz of the carbons and heteroatoms in molecule and the 1s orbitals of the hydrogen atoms. These orbitals form the basic set. When this basic set contains only the atomic-like orbitals for the valence shell of the atoms in a molecule, it is called a minimal basic set.

Each φ_j, with $j = 1 \dots N$, represents a molecular orbital, i.e. the wave function for one electron moving in the electrostatic field of the nuclei and the other electrons. Two electrons with different spins are placed in each molecular orbital so that the number of occupied molecular orbitals *N* is a half a number of electrons, *n*, i.e. $N = n/2$.

The number of molecular orbitals that one obtains by this procedure is equal to the number of atomic orbitals. Consequently, the indices *j* and *r* both run from 1 to *N*. The c_{jr} are the weighting coefficients of the atomic orbitals in the molecular orbital. These coefficients are not necessarily equal, or in other words, the orbital on each atom is not used to the same extent to form each molecular orbital. Different values of the coefficients lead to different net charges at different positions in a molecule. This charge distribution is very important when spectroscopy and chemical reactivity are discussed.

The energy of the j^{th} molecular orbital is given by a one-electron Schrödinger equation using an effective one electron Hamiltonian, h_{eff}, which expresses the interaction of an electron with the rest of the molecule.

$$h_{eff}\psi_j = \epsilon_j\psi_j \tag{5}$$

ϵ_j is the energy eigenvalue of the j^{th} molecular orbital, corresponding to the Eigen function $\psi_j\psi_j$. The beauty of this method, as we will see later, is that the exact form of h_{eff} is not needed. The total energy of the molecule is the sum of the single electron energies.

$$E_\pi = \sum_j n_j \epsilon_j \tag{6}$$

where n_j is the number of electrons in orbital j.

The expectation value expression for the energy for each molecular orbital is used to find ϵ_j and then E_π

$$\epsilon_j = \frac{\int \psi_j \times h_{eff} \psi_j d\tau}{\int \psi_j \times \psi_j d\tau} = \frac{\langle \psi_j | h_{eff} | \psi_j \rangle}{\langle \psi_j | \psi_j \rangle} \tag{7}$$

After substituting Equation (6) into (7), we obtain for each molecular orbital

$$\epsilon_j = \frac{\langle \sum_{r=1}^{N} c_{jr} \varphi_r | h_{eff} | \sum_{s=1}^{N} c_{js} \varphi_s \rangle}{\langle \sum_{r=1}^{N} c_{jr} \varphi_r | \sum_{s=1}^{N} c_{js} \varphi_s \rangle} \tag{8}$$

It can be rewritten as

$$\epsilon = \frac{\sum_{r=1}^{N} \sum_{s=1}^{N} c_r^* c_s \langle \psi_r | h_{eff} | \psi_s \rangle}{\sum_{r=1}^{N} \sum_{s=1}^{N} c_r^* c_s \langle \psi_r | \psi_s \rangle} \tag{9}$$

where the index j of the molecular orbital was dropped because this equation applies to any of the molecular orbitals. [3]

3.2 Density Function Theory

Currently Density Function Theory (DFT) is the most successful approach to compute molecular structure but it is much slower than Extended Hückel method, so I will use DFT only for final calculation to get more precise results.

The conventional approaches use the wave function Ψ as the central quantity, when Ψ contains the full information of a system. However, Ψ is a very complicated quantity that cannot be probed experimentally and depends on *4 N* variables, where *N* is number of electrons in system.

However, the electron density is observable and can be measured experimentally (e.g. by X-ray diffraction).

The first Hohenberg-Kohn theorem demonstrates that the electron density uniquely determines the Hamiltonian operator and thus all the properties of the system. This first theorem states that the external potential $V_{ext}(\vec{r})$ is a unique functional of $\rho(\vec{r})$; in turn $V_{ext}(\vec{r})$ fixes $\hat{H}$ and we see that the full many particle ground state is a unique functional of $\rho(\vec{r})$. It makes the electron density the central quantity in DFT. It can be

defined as the integral over the spin coordinates of all electrons and over all but one of the spatial variables

$$\rho(\vec{r}) = \int \dots \int |\Psi(\overrightarrow{x_1}, \overrightarrow{x_2}, \dots, \overrightarrow{x_n})|^2 ds_1 \, d\vec{x}_1 \dots d\vec{x}_n \tag{10}$$

$\rho(\vec{r})$ defines the probability of finding any of the N electrons within volume element $d\vec{r}$ ($\vec{r} \equiv \vec{x}$).

Focusing on the electron density, it is possible to derive an effective one-electron-type Schrödinger equation and also all type of correlation energy in solid body:

- Ion-electron potential energy
- Ion-ion potential energy
- electron-electron energy
- kinetic energy
- exchange-correlation energy

To make calculation much faster and easier, as 1st step of DFT we must reduce as far as possible the number of degrees of freedom of the system. It can be done according to Born-Oppenheimer approximation.

The main idea of this approximation is that the kinetic energy of the ions is much smaller than of the electrons. The electrons are assumed to respond instantaneously to the motion of the ions. For any ionic configuration we assume that the electrons are in the instantaneous ground-state and calculate the total energy of the system. Varying the ionic positions defines a multi-dimensional ground-state potential energy surface, and the motion of the ions can then be treated as classical particles moving in this potential.

$$\hat{\mathrm{H}}_{elec} \Psi_{elec} = E_{elec} \Psi_{elec} \tag{11}$$

The total energy E_{tot} is the sum of E_{elec} and the constant nuclear repulsion term E_{nuc}.

Focusing on the electron density, it is possible to derive an effective one-electron-type Schrödinger equation.

From electron density function we can derive:

- Ion-electron potential energy
- Ion-ion potential energy
- Electron-electron energy
- Kinetic energy

It is almost everything we need to have a good picture of the electron transport inside our device.

3.3 Tight Binding Model

The last thing but not the least I wanted to mention in 1st part of this work is Tight Binding Model (TB model). This model is simplification, which provides faster calculation with negligible error. TB model is an approach to the calculation of electronic band structure using an approximate set of wave function at each atomic site.

The simplest model of electrons moving through a crystal is the so-called "tight-binding chain", which involves electrons that are bound to atomic orbitals at each site of the crystal lattice hopping between neighboring sites. This model only seems very simple. To describe this more precisely let's assume that in 1D system of atoms, where every atom has only one orbital, label the orbital for the electron sitting at atom *n* as $|n\rangle$. They are taken to be orthogonal (not really orthogonal, but atoms are far away enough from each other to say that their wave function is not overlapped),

$$\langle n|m\rangle = \delta_{n,m} \tag{12}$$

where $\delta_{n,m}$ is the Kronecker delta.

We can write the state of the electron in the basis of the orbitals

$$|\varphi\rangle = \sum_n c_n|n\rangle \tag{13}$$

The time-independent Schrödinger equation then can be written in the basis of these orbitals as

$$\sum_n H_{nm}c_m = Ec_n \tag{14}$$

The Hamiltonian only couples nearest neighbor sites, so we can write

$$\langle n|H|m\rangle = \begin{cases} \varepsilon_0, & n = m \\ -J, & n = m \pm 1 \\ 0, & otherwise \end{cases} \tag{15}$$

Where ε_0 is the zero-point energy of each bound orbital (and is the same at each site of the crystal), and $-J$ indicated how rapidly the electron hops (probability of hopping).

Then we can write energy function of 1D system:

$$E = \varepsilon_0 - 2Jcos(ka) \tag{16}$$

Where k is momentum (wave vector) and includes dependence on the distance between atoms.

4. Simulation of GNR on SiC

4.1. Virtual NanoLab with Atomistix ToolKit

Virtual NanoLab with Atomistix ToolKit is a general-purpose atomic-scale modeling and simulation platform, which combines a wide range of methods and models.[10]

Atomistix ToolKit (ATK) is a software package with the most complete set of tools for atomistic simulations. ATK can compute electronic, optical, thermal, mechanical, and other properties of nanostructures and materials. In addition, ATK can perform electron transport and analysis of nanoscale devices, both in the ballistic tunneling regime and taking electron-scattering into account. The code also provides a state-of-the-art molecular dynamics engine. ATK is also the market leading software for electronic transport calculations. ATK is benefiting from the graphical user interface, which is called Virtual NanoLab.

Virtual NanoLab (VNL) is an easy-to-use graphical user interface, which makes it simple to carry out tasks, while a Python programming interface allows experienced users to efficiently implement complex work-flows and perform advanced data analysis. VNL can also act as a standalone interface to other codes, with capabilities to build geometries and set up calculations, and read and plot output results produced by VASP, LAMMPS, ABINIT, QuantumEspresso, etc. Users can furthermore extend the capabilities and interfaces of the package by implementing their own plugins to support additional file formats, combine and plot data in other ways, set up new types of structures, etc. [10]

The whole practical section can be divided into 3 parts. In the first part we are going to build the nanostructure using VNL Builder (Figure 4.1.1). The Stash displays the structures you are working on in the Builder, in the menu; you can choose one of the options to create a new build: new configuration, from files, from database, from plugin, from clipboard. The most common options are “add from database”, “add from files” and “add from plugin”. The option “add from database” opens the built-in database of ATK with thousands of molecules, crystals and fullerenes, which can be used directly in your calculations. The option “add from files” you can use when you want to import something you built earlier, or perhaps a file you downloaded from an online database

or generated in other software. If you want to work with graphene or nanotubes you can find some useful plugins for this by choosing option “add from plugin”. Nanotube, nanoribbon and nanosheet are default options but the list can be extended by plugin manager. The default data type, which is used for saving the geometry, is ATK python. Stash items can be both selected and active but only one stash item can be active. This is the structure shown in the 3D window. At this step you can also use optimizer, to optimize geometry and find the position of each atom with minimal energy force; it also reduces the time of calculations during the next step.

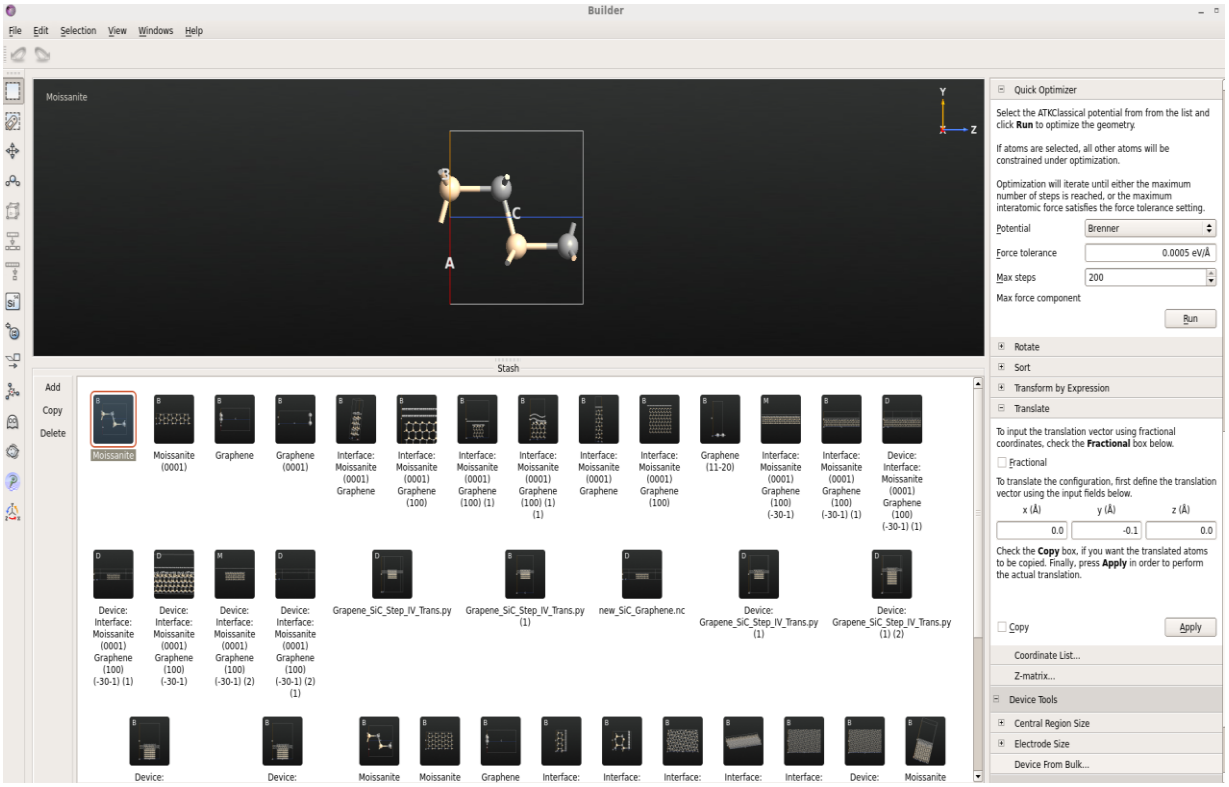

Figure 4.1.1: Virtual NanoLab Bilder

When you finish with geometry, you can move to the next step: script setup (Figure 4.1.2). VNL allows you to focus on physics instead of programming. In script generator we can define the method, a calculator to use, configure its parameters and select the physical properties to compute. The calculator has default options for all parameters however you should always check them carefully in order to obtain the desired accuracy, and to determine which method should be used. The default method is the DFT, but this method requires relatively long time to execute. The next option is to use semi empirical extended Hückel method. The next thing you can set up is k-point sampling, which allows tuning the proper accuracy. The other features I will describe in

the next chapter. The second thing we should know about Script Generator is a list of analysis. It is possible to choose the output of your scripts from this list.

You can execute the script using job manager or command line. After the job is finished, we can move to the 3rd step: analysis of the result.

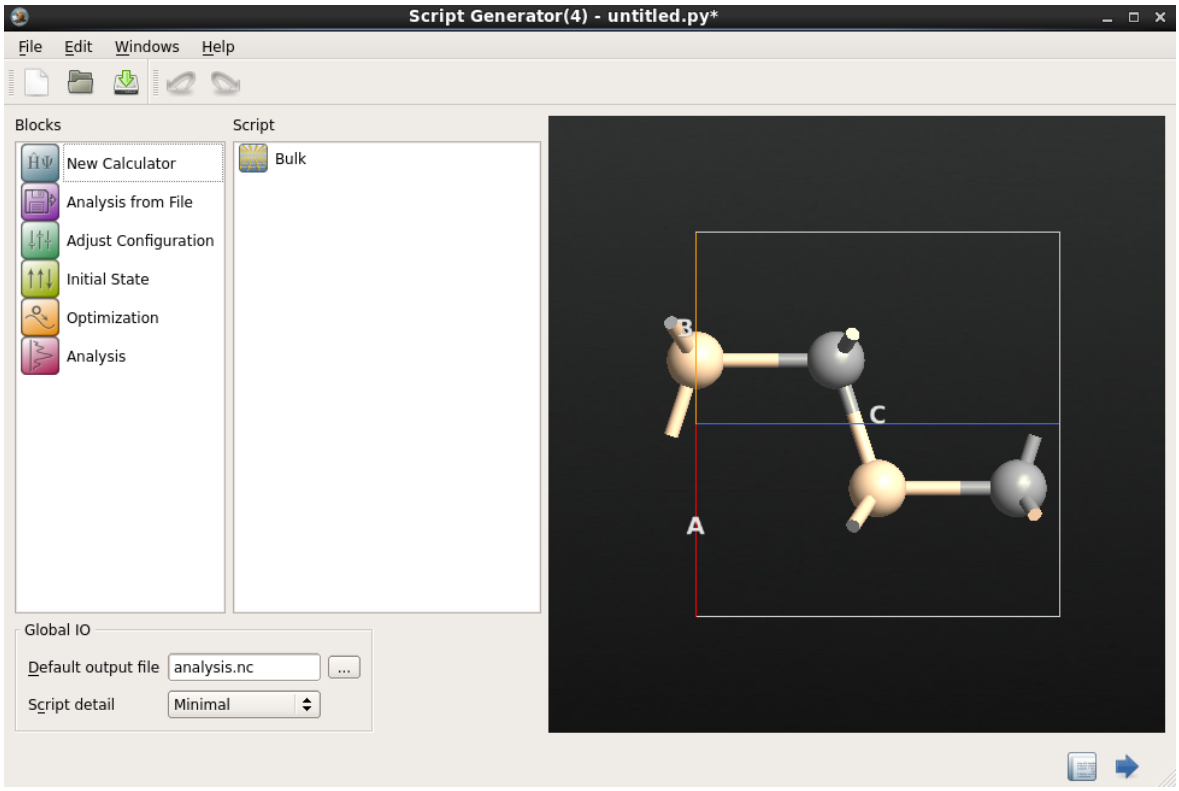

Figure 4.1.2: Interface for script setup.

4.2. Building the Geometry

In this work we consider 2 different structures: graphene on step shape SiC substrate and graphene on planar substrate with additional interface graphene layer. All molecules were taken from standard VNL database. As substrate we use Moissanite (SiC), because of its hexagonal crystal system. The primitive cell you can see on Figure 4.2.1

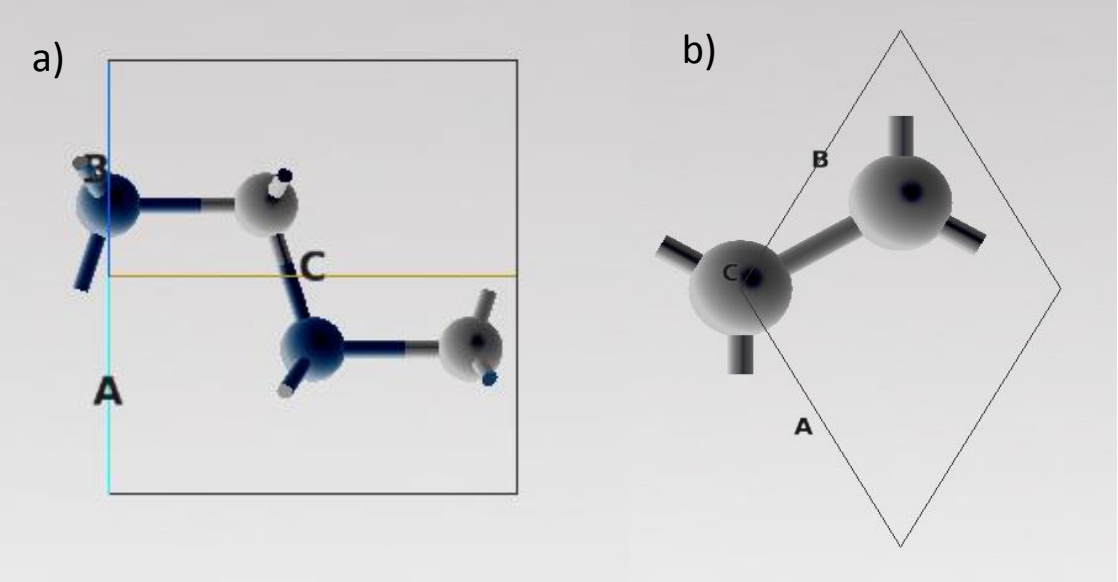

Figure 4.2.1:
a) The primitive cell of Moissanite (SiC)
A = 3.076 Å C = 5.048 Å
b) The primitive cell of Graphene
A = 2.4612 Å C = 6.709 Å

We also choose graphene molecule in the database. Primitive cell of graphene you can see on Figure 4.2.1(b). Then you can create interface between two surfaces (Figure 4.2.2).

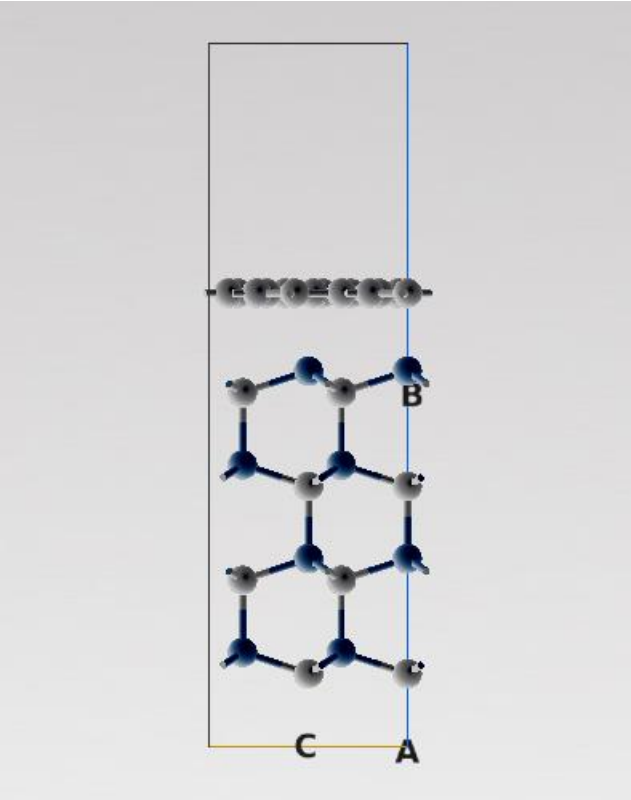

Figure 4.2.2: The interface between graphene and SiC.

Relying on Figure 2.9.1 we need second graphene layer. We also need to extend our structure for future device (we need at least 3 periods of super lattice to define contacts and central region). Because of some stochastic behavior of the graphene on SiC, the covalent bonds between layers have no period and after optimization it becomes even worst. So the problem is that at the end we will have very long structure with thousands of atoms. To avoid such problem we need to create the device directly from initial bulk and then do all optimization and passivate structure by hydrogen. The distance between the first layer of graphene and SiC substrate is equal to ≈1.43 Å, this value is given differently in different paper, so the main criteria was the maximum distance on which we could get covalent bonds between the layers. The distance between the first and the second graphene layer is equal to 2.7 Å on this distance.

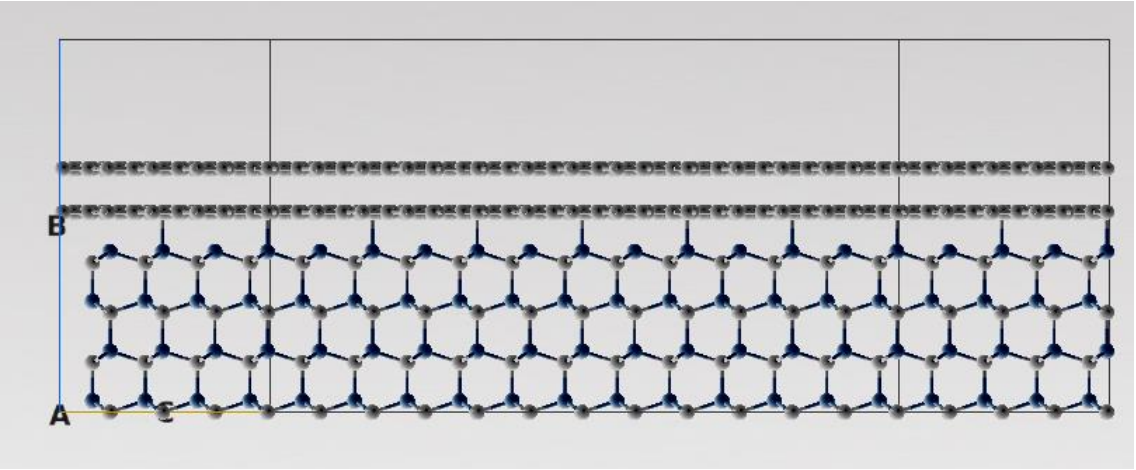

Figure 4.2.3: Planar structure of graphene.

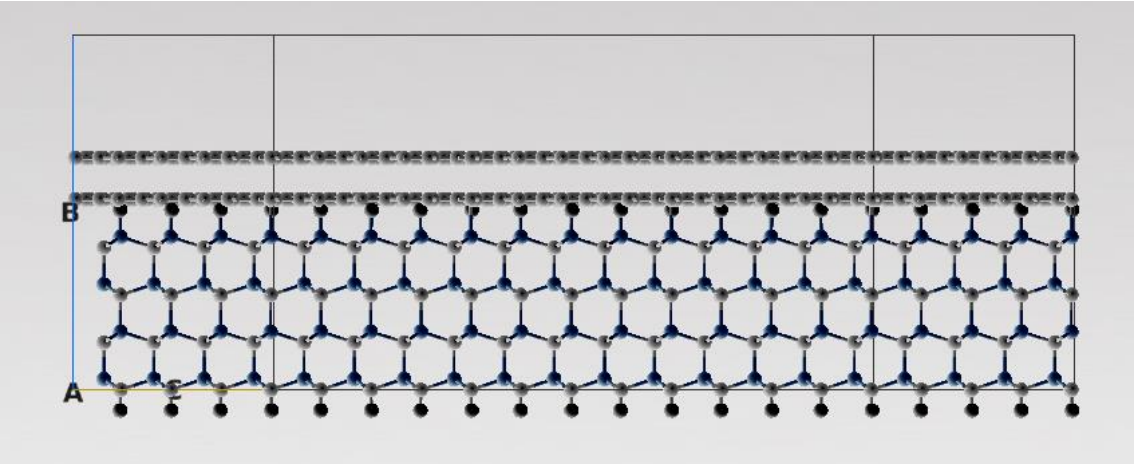

Figure 4.2.4: Planar structure of graphene after passivation by hydrogen.

The next structure we are focused on is graphene on step shape SiC. The main problem here is to save proper structure of SiC and graphene. Because of the different lattice constant, it is very difficult to make sure that structure is periodic in all directions. We have to reduce a number of atoms as much as possible to minimize the time of calculations. So graphene was a little bit stretched. Then the structure was also passivated by hydrogen and optimized by minimization of Brenner potential. In the case with planar structure the minimum max force component was reached is 1.0899 eV/Å, for step structure it is 3.3424×10^{-4} eV/Å.

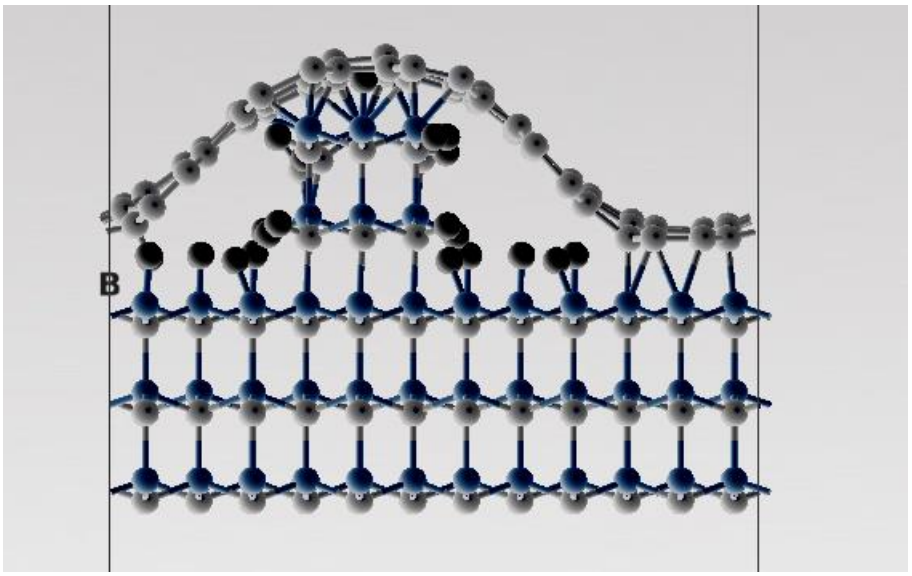

Figure 4.2.5: Graphene on step shape SiC.

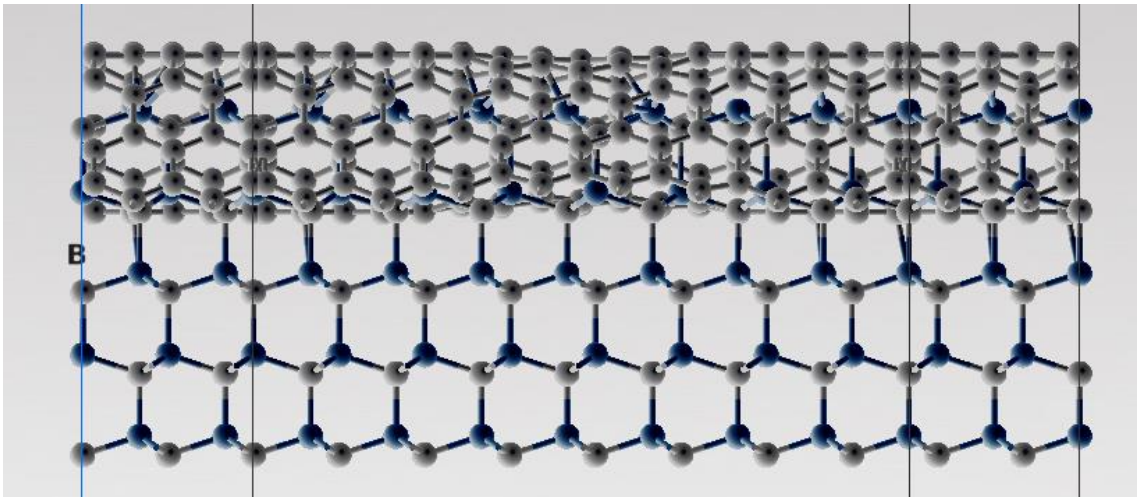

Figure 4.2.6: Graphene on step shape SiC.

As you can see on the Figure 4.2.6, SiC crystal structure is ideal periodic. For graphene lattice is not the same. At junction, there are some impurities, but the middle part is the proper graphene we are looking for.

4.3. Script Generation

In both cases we use Extended Hückel model, in order to minimize the time of calculation and at the same time to have enough precise results. As elements we use Cerda.Carbon[graphite] with vacuum level -7.36577 eV, Cerda.Hydrogen[C_2H_4] with

vacuum level -6.2568 eV and Cerda.Silicon [GW SiC] with vacuum level -6.14175, due to Quantum wise manual recommendation. To get proper accuracy we put k-point sampling in a following way:

n_A = 10, n_B = 3 and n_C = 100 for flat structure and n_A = 4, n_B = 4 and n_C = 100 for step structure. We picked these values empirically trying to find middle ground between the accuracy and the time of the computation. As a Poisson equation solver we choose FFT2D, which use periodic boundary conditions in front, back, bottom, top and Dirichlet in left and right. Also we need to make sure that periodic condition in top and bottom direction does not affect our structure by extending the cell borders respectively. Two main analyzes we use in this work are TransmissionPathways and IVCurve.

Settings for TransmissionPathways are:

1) Energy = 0 eV
2) Infinitesimal 1e-06 eV
3) Self-energy calculator: Direct
4) Energy zero parameter: Average Fermi level
5) Contributions: Left

For IVCurve are:

1) Voltage Bias: V_0 = 0; V_1 = 0.2; Points = 4;
2) Energy: E_0 = -2; E_1 = 2; Points = 101
3) Energy zero parameter: Average Fermi level
4) Infinitesimal: 1e-6 eV
5) Self-energy calculator: Recursion

The created scripts are attached to this thesis as Appendix B, and Appendix C and can be used to continue this work from the last reached point.

4.4. Results

Firstly, we get results for planar not passivated structure and it is not satisfactory. Even if structure is symmetric without any defects, existing of free bonds has a huge effect on results. On Figure 4.4.1 you can see transmission pathways for this structure.

On this diagram the thickness of lines represents scaled transmission t_{sc} and calculated by following formula:

$$t_{sc} = \frac{t}{t_{max}} p$$

where t is a transmission, t_{max} is a maximum transmission, p is a scale coefficient, which was found empirically and in most cases is equal to 0.25. For each calculation t_{max} is different and we cannot compare these results.

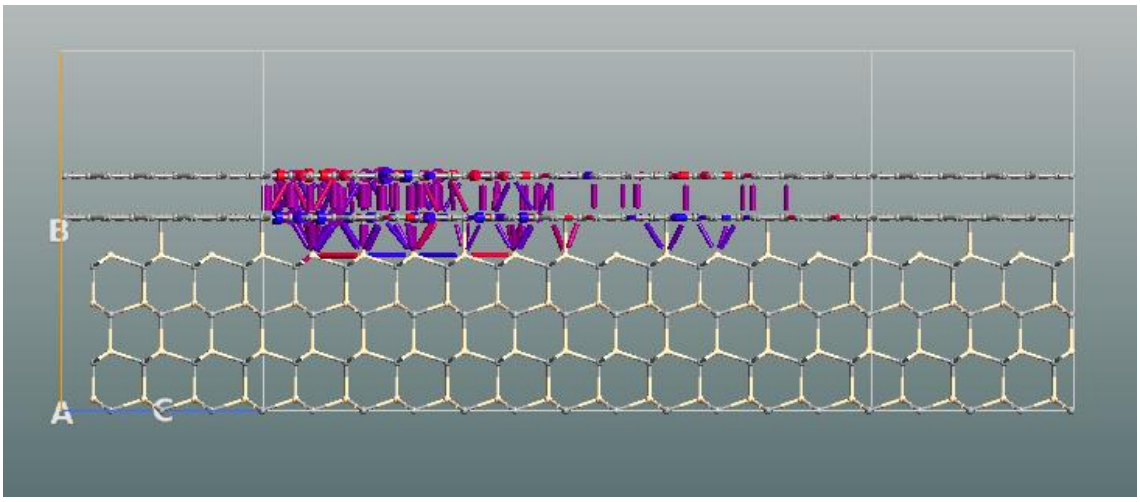

Figure 4.4.1: Transmission pathways of flat graphene on SiC structure.

The states density is distributed not uniformly, and it makes me think that this structure does not have right behavior and we can remove it from further discussion.

So we can move to the passivated planar structure. On the Figure 4.4.2 you can see its transmission pathways diagram.

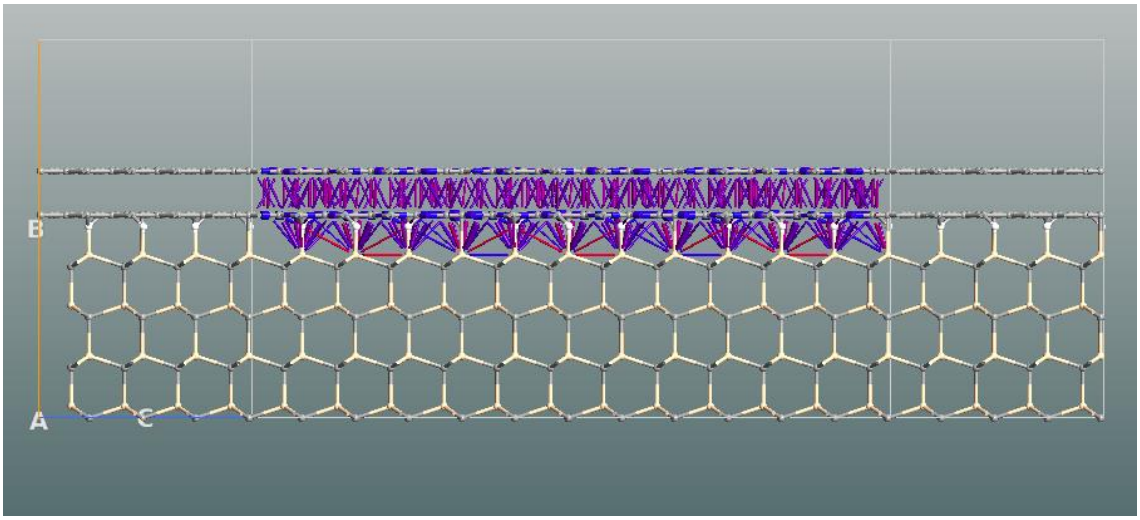

Figure 4.4.2: Transmission Pathways in passivated graphene on SiC

On Figure 4.4.2 we can see that no current goes through SiC, because SiC has a band gap at Fermi level of energy (see Figure 4.4.3). On the other hand, we can see that graphene at this energy behaves as conductor. As we know from [5] SiC, substrate can have influence on a band gap in graphene. The reason, why we do not see it here, is that during the calculation the software uses only one zero energy, while for silicon carbide and graphene they are different. In our model the amount of SiC is greater than of graphene, so SiC dominates over graphene. Transmission pathways analysis does not provide the information where band gap can be found and how big it is. Looking on Figure 4.4.2 we can say that the most current will travel in second graphene layer, the first graphene layer does not behave as graphene but together with topsheet of silicon carbide creates buffer layer.

IV characteristic (Figure 4.4.4) is almost linear with coefficient 0.12 S. On the Figure 4.4.5 there is a non-zero transmission function; so we can assume that there is band gap on the energy -1 eV, where transmission is equal to 2.06×10^{-9}.

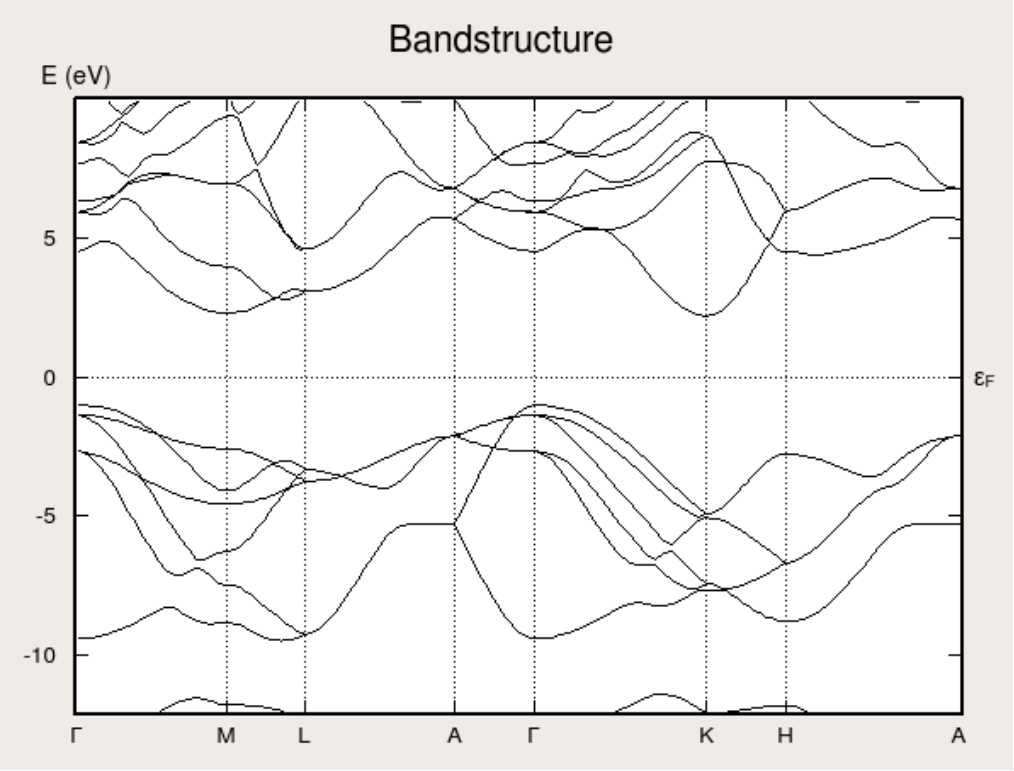

Figure 4.4.3: Bandstructure of SiC

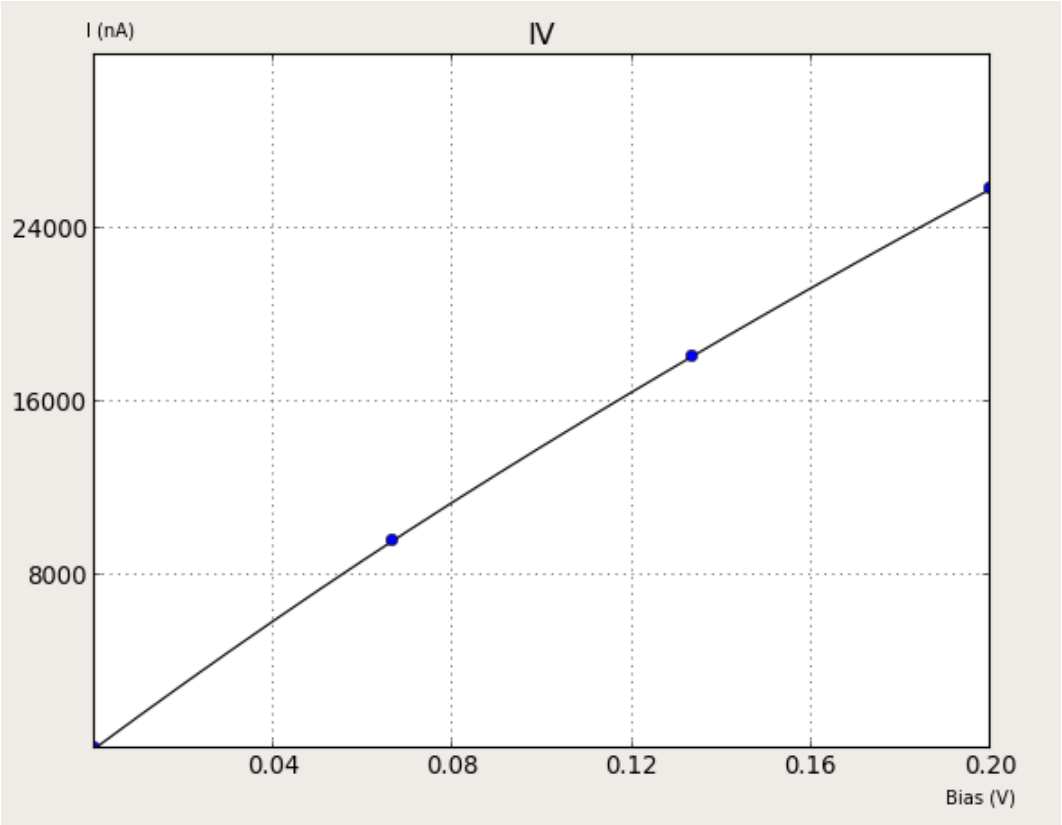

Figure 4.4.4: IVCurve of graphene on flat surface of SiC

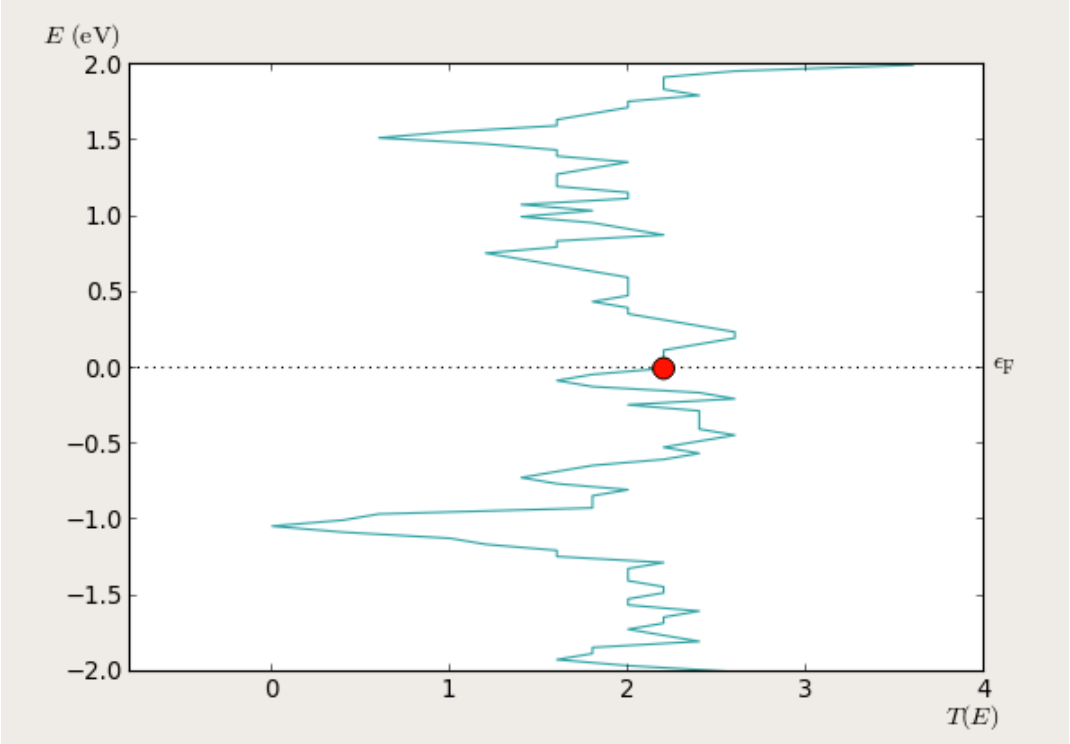

Figure 4.4.5: Transmission function of graphene on flat surface of SiC

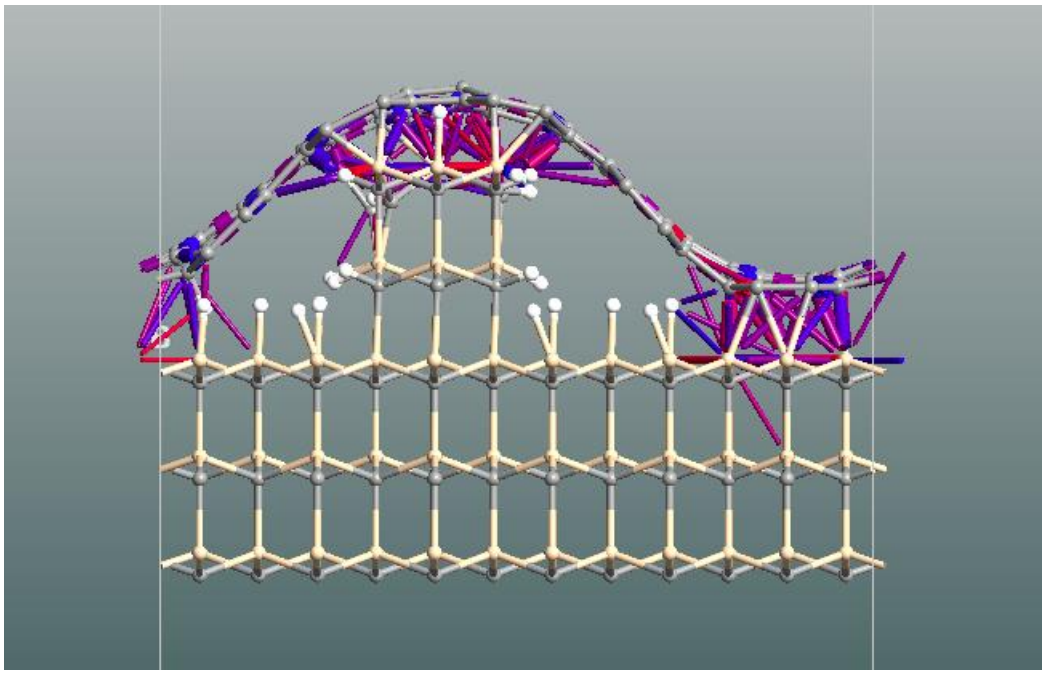

Figure 4.4.6: Transmission pathways in graphene on step shape SiC

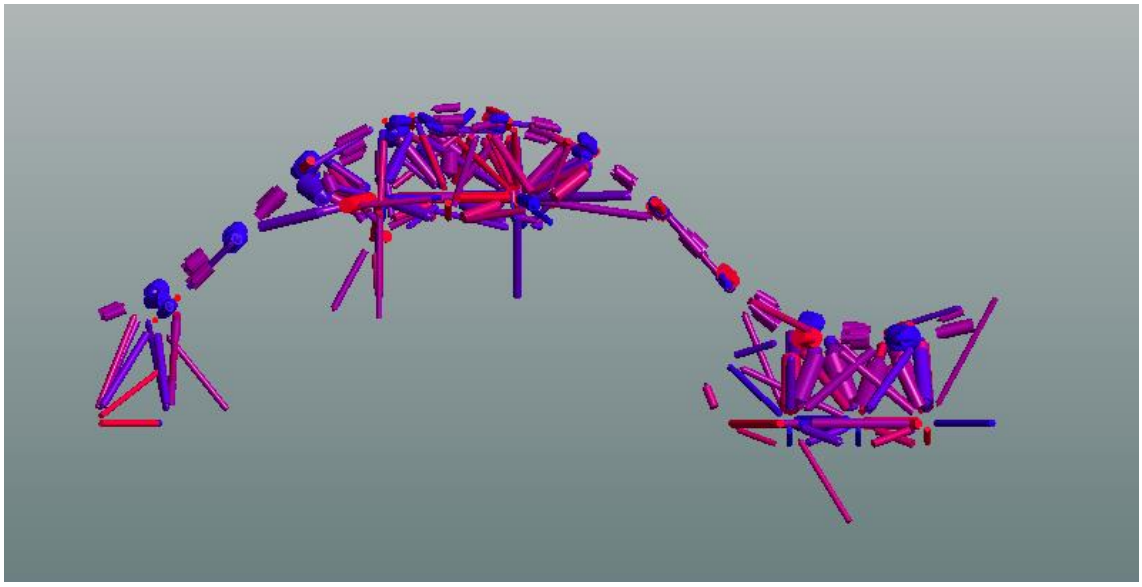

Figure 4.4.7: Transmission pathways in graphene on step shape SiC

Now we can move to the other structure – graphene on facet. On the Figure 4.4.5 we can see that in the flat regions of SiC graphene behaves in the same way as first layer in previous case, but graphene on facet is free nanoribbon, it has interaction only with side graphene.

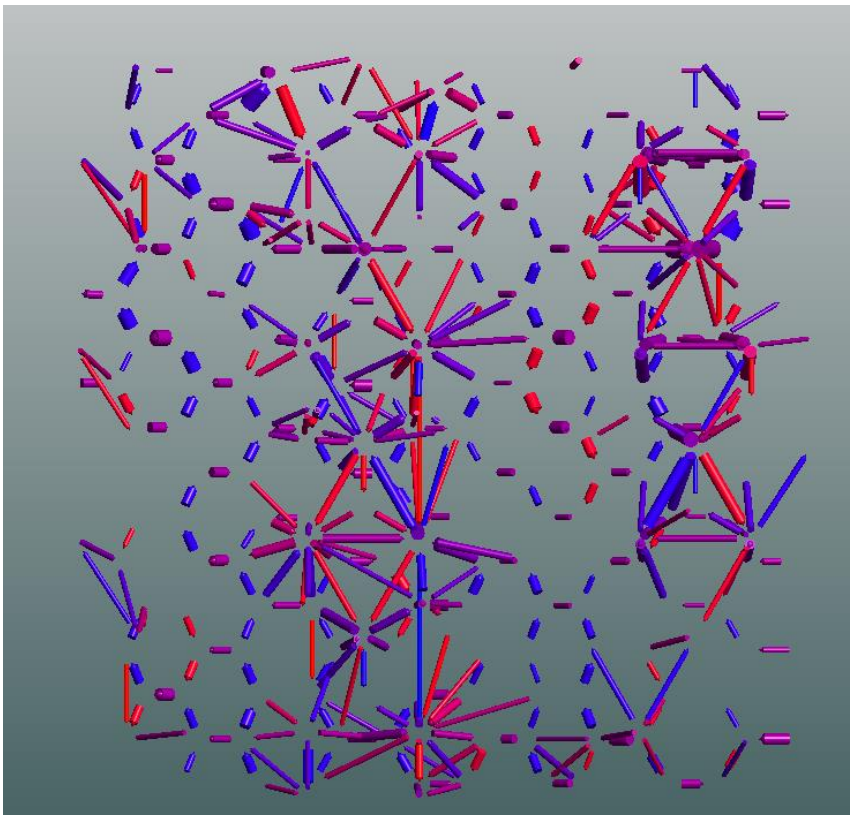

Figure 4.4.8: Transmission pathways in graphene on step shape SiC (top view)

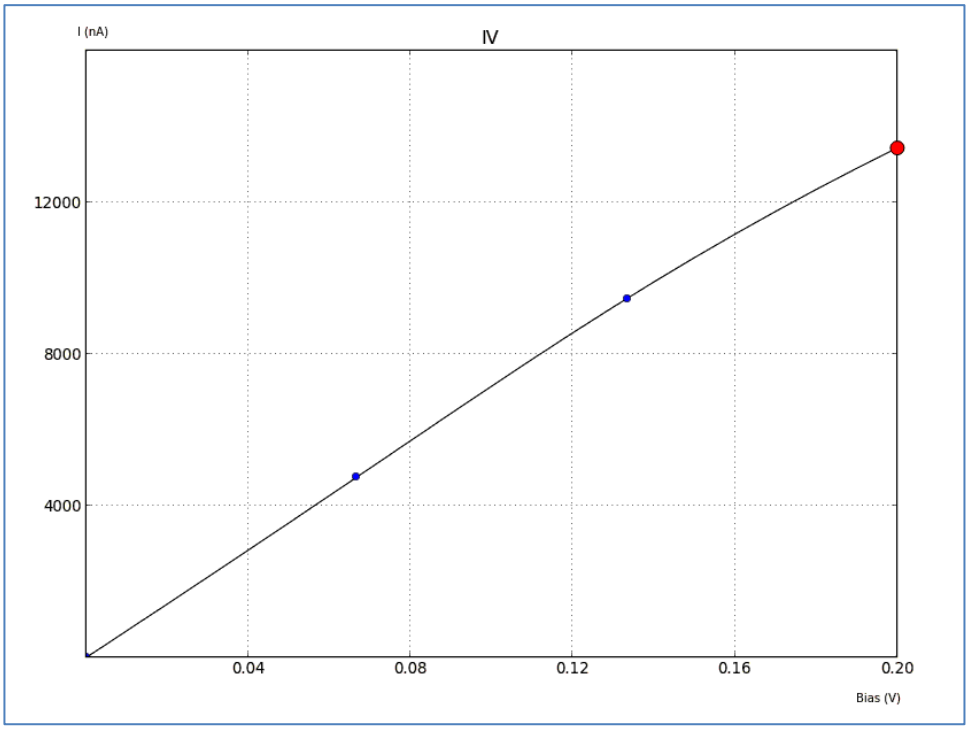

Figure 4.4.9: IV curve of graphene on step shape SiC

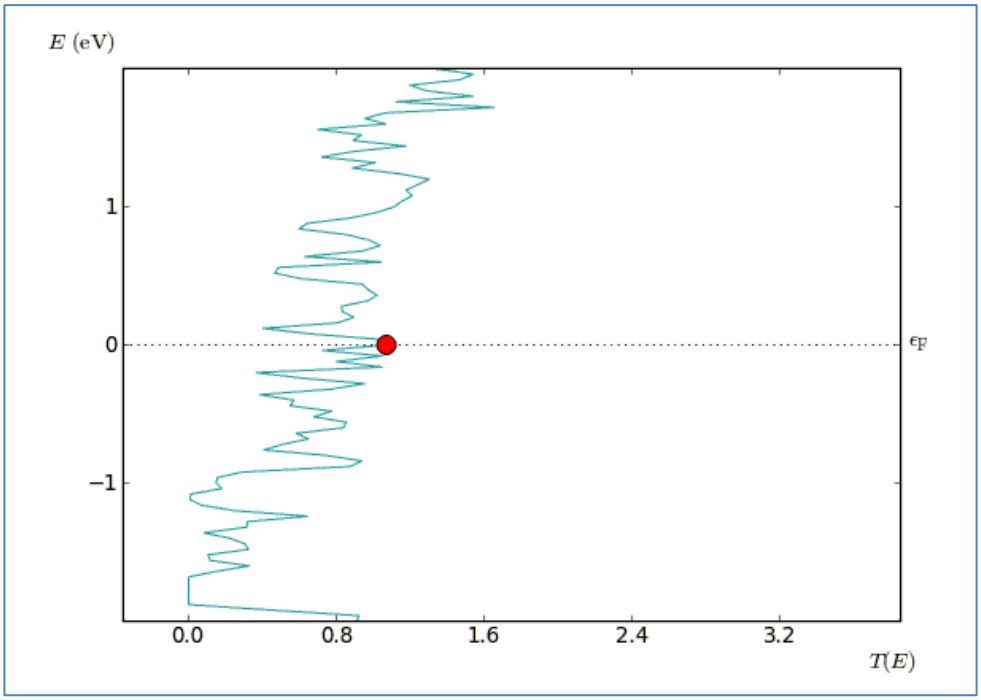

Figure 4.4.10: Transmission function of graphene on etched surface of SiC

The coefficient of this IV curve is around 0.075 S, which is almost twice less than for flat structure.

On Figures 4.4.11 – 4.4.14 there are results of the transmission pathways analysis of step structure on different energies (-1, -0.5, 0.5, 1). Looking on them we can say that on energies higher than 1 silicon carbide is conductive, it describes behavior of IV curve above 1 eV (for clarity see Figure 4.4.15).

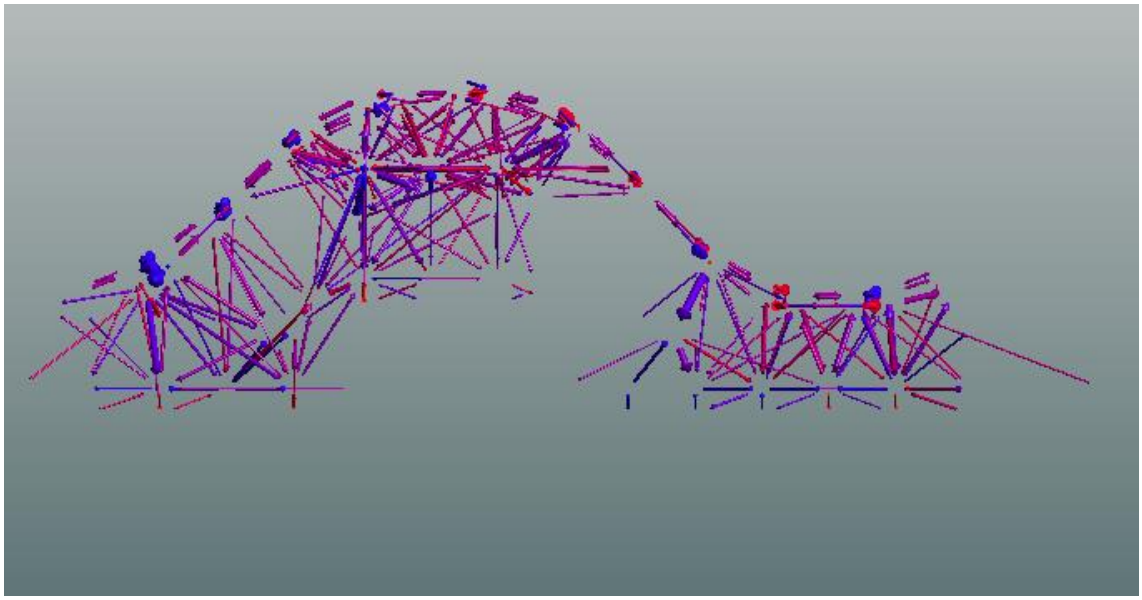

Figure 4.4.11: Transmission Pathways of step structure on energy = -1 eV

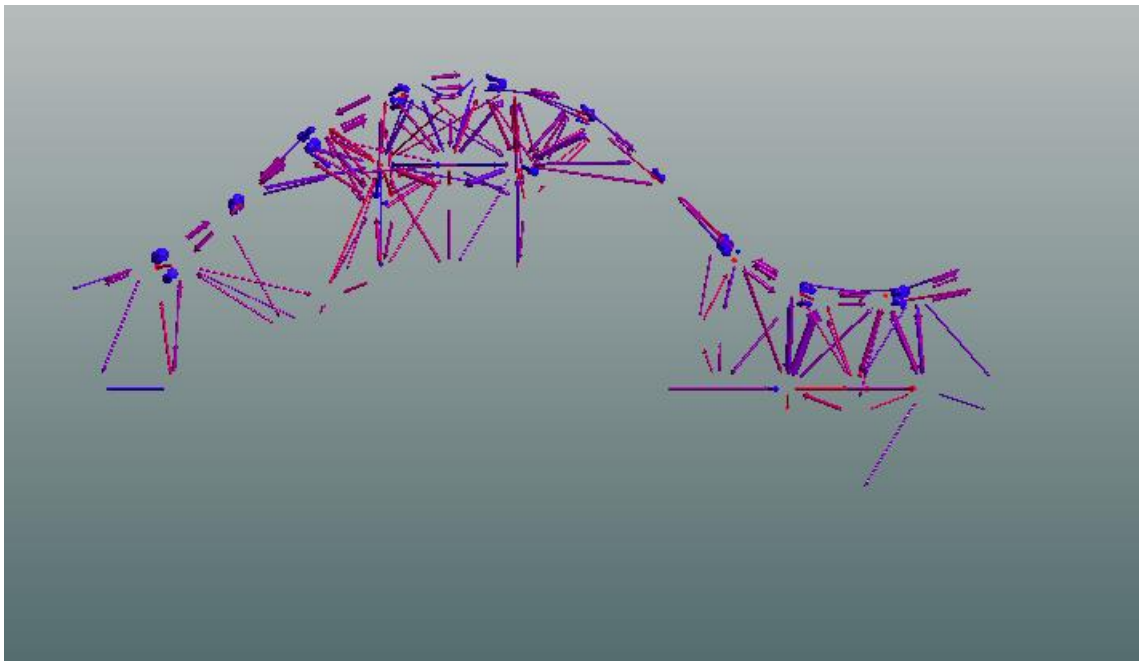

Figure 4.4.12: Transmission Pathways of step structure on energy = -0.5 eV

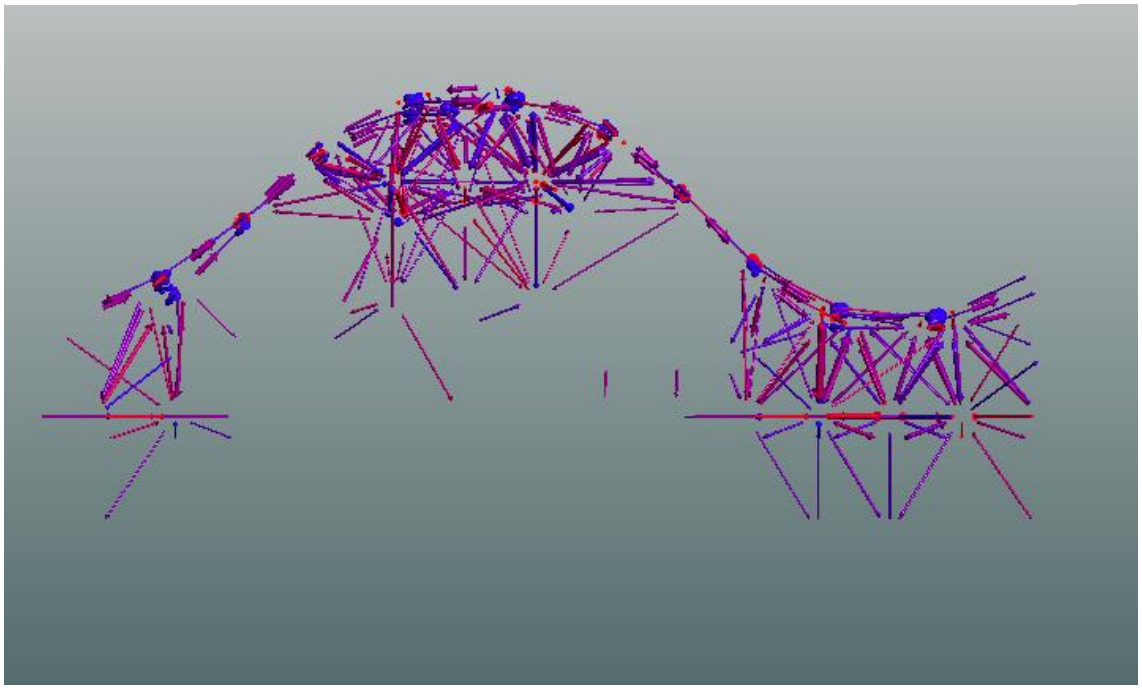

Figure 4.4.13: Transmission Pathways of step structure on energy = 0.5 eV

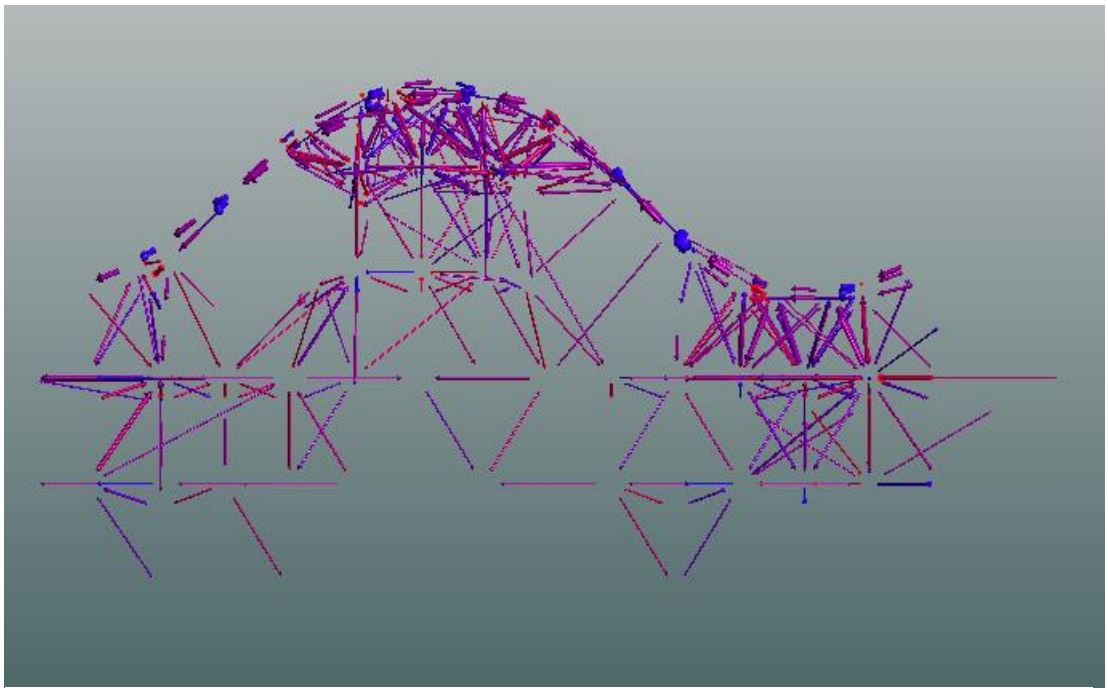

Figure 4.4.14: Transmission Pathways of step structure on energy = 1 eV

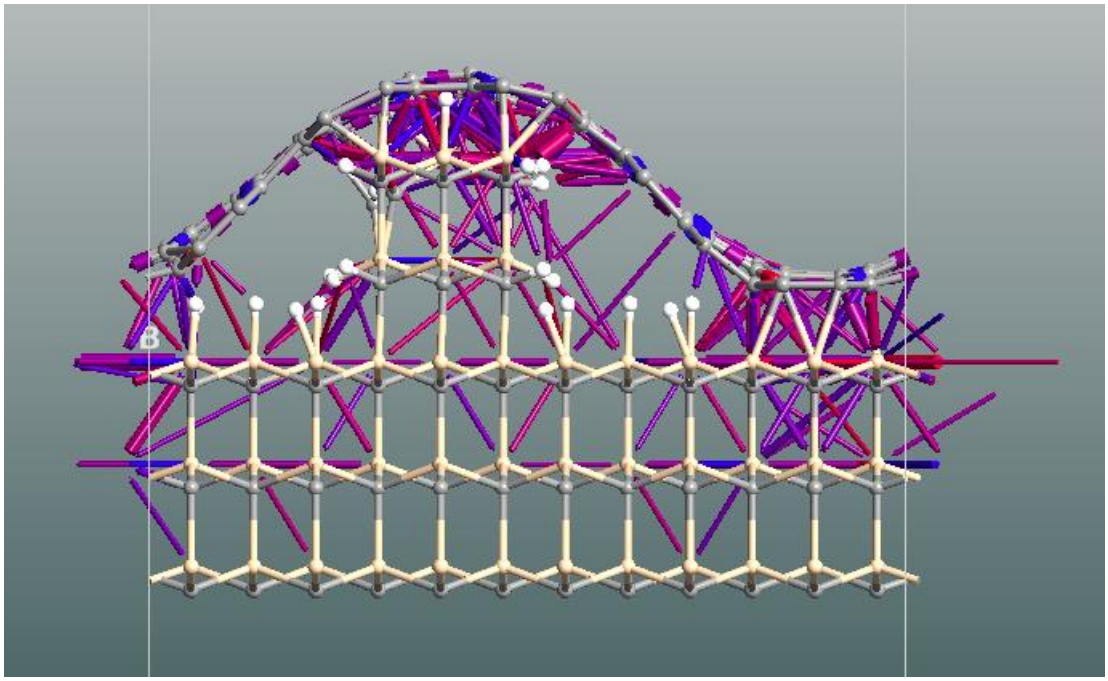

Figure 4.4.15: Transmission Pathways of step structure on energy = 1 eV with device structure

5. Conclusion

In the theoretical part of my thesis, the graphene technologies state of art was summarized. I concentrated on the area of graphene layers and nanoribbons on silicon carbide. I studied such things like influence of silicon carbide substrate on graphene bandpass structure, influence of hydrogenation and dependence on face of substrate. The experimental results showed the advantage of the placement of the graphene nanoribbon on the facet etched on the wafer surface in comparison with the placement on the flat structure. Produced graphene had better mobility and larger mean free path of electron transport.

Both above mentioned structures were created in practical part. Obtained results were compared with experimental data. The transmission property was selected to evaluate the accuracy. We can look more precisely at resistivity of the graphene nanoribbon. Experimental data from article [11] give us a value 26 kΩ for graphene sample 1.6 μm length and 39 nm width. If we take into account that our step structure model is 1000 times shorter and 20 times narrower, our value of resistance (13 Ω) has the same order but still a little bit less than experimental one. The reason is that we are not taking into account the electron-phonon collisions, temperature of environment and other unideal conditions which we can meet in real life. By the way, obtained results have enough accuracy to continue working with created model and investigate other properties, which are not testable or very expensive to measure by real experiment. In my work basic analysis of graphene nanostructure on step shape silicon carbide is presented and these data can be used for continuous investigation which is beyond boundary of this thesis.

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Appendix A

Table 1 *Silicon Carbide Material Properties*

Mechanical	Value (SI/Metric)
Density	3.1 gm/cc
Porosity	0%
Color	Black
Flexural Strength	550 MPa
Elastic Modulus	410 GPa
Poisson's Ratio	0.14
Compressive Strength	3900 MPa
Hardness	2800 Kg/mm^2
Fracture Toughness K_{IC}	4,6 $MPa*m^{1/2}$
Maximum Use Temperature	1650˚C
Thermal	
Thermal Conductivity	120 W/m*˚K
Coefficient of Thermal Expansion	$4.0 * 10^{-6}$/˚C
Specific Heat	750 J/Kg*˚K
Electrical	
Volume Resistivity	10^2-10^6 ohm*cm

Appendix B

```
# ------------------------------------------------------------
# TwoProbe configuration
# ------------------------------------------------------------

# ------------------------------------------------------------
# Left electrode
# ------------------------------------------------------------

# Set up lattice
vector_a = [6.152, 0.0, 0.0]*Angstrom
vector_b = [0.0, 18.905, 0.0]*Angstrom
vector_c = [0.0, 0.0, 10.6555765682]*Angstrom
left_electrode_lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
left_electrode_elements = [Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                           Silicon, Silicon, Carbon, Carbon, Silicon, Silicon, Carbon,
                           Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Hydrogen,
                           Hydrogen, Hydrogen, Hydrogen, Carbon, Carbon, Silicon, Silicon,
                           Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon,
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# Define coordinates
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[4.613999999997, 0.580519999998, 9.614718268257],
[1.537999999997, 2.524000000004, 9.614718268257],
[4.613999999997, 2.524000000004, 9.614718268257],
[1.537999999997, 5.628520000005, 9.614718268257],
[4.613999999997, 5.628520000005, 9.614718268257],

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                        [  1.537999999997,   7.571999999992,   9.614718268257],
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                        [  2.197142857141,  10.152519999999,   9.741570370251],
                        [  2.197142857141,  12.852519999999,   9.741570370251],
                        [  3.515428571428,  10.152519999999,   9.995274574261],
                        [  3.515428571428,  12.852519999999,   9.995274574261],
                        [ -0.000000000003,   0.            ,  10.50268298227 ],
                        [  3.075999999997,   0.            ,  10.50268298227 ],
                        [ -0.000000000003,   3.104520000002,  10.50268298227 ],
                        [  3.075999999997,   3.104520000002,  10.50268298227 ],
                        [ -0.000000000003,   5.048000000007,  10.50268298227 ],
                        [  3.075999999997,   5.048000000007,  10.50268298227 ],
                        [ -0.000000000003,   8.152520000009,  10.50268298227 ],
                        [  3.075999999997,   8.152520000009,  10.50268298227 ],
                        [ -0.000000000003,  10.152519999999,  10.50268298227 ],
                        [ -0.000000000003,  12.852519999999,  10.50268298227 ],
                        [  0.007326711628,  -1.089252078357,  10.542382587151],
                        [  3.083326711628,  -1.089252078357,  10.542382587151],
                        [  3.085612107913,   9.581538781708,  10.55476595012 ]]*Angstrom

# Set up configuration
left_electrode = BulkConfiguration(
    bravais_lattice=left_electrode_lattice,
    elements=left_electrode_elements,
    cartesian_coordinates=left_electrode_coordinates
    )

# ------------------------------------------------------------
# Right electrode
# ------------------------------------------------------------

# Set up lattice
vector_a = [6.152, 0.0, 0.0]*Angstrom
vector_b = [0.0, 18.905, 0.0]*Angstrom
vector_c = [0.0, 0.0, 10.6555765682]*Angstrom
right_electrode_lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
right_electrode_elements = [Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                        Silicon, Silicon, Carbon, Carbon, Silicon, Silicon, Carbon,
                        Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Hydrogen,
                        Hydrogen, Hydrogen, Hydrogen, Carbon, Carbon, Silicon, Silicon,
                        Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon,
                        Carbon, Carbon, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon,
                        Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                        Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Silicon,
                        Silicon, Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen, Carbon,
                        Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Silicon,
                        Silicon, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon,
                        Carbon, Carbon, Carbon, Carbon, Carbon, Hydrogen, Hydrogen,
                        Hydrogen, Hydrogen, Carbon, Carbon, Silicon, Silicon, Carbon,
```

```
                    Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Silicon,
                    Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Silicon, Silicon, Carbon, Carbon, Silicon, Silicon,
                    Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen]

# Define coordinates
right_electrode_coordinates = [[  1.318285714281,  10.152519999999,   0.10081061808 ],
                               [  1.318285714291,  12.852519999999,   0.10081061808 ],
                               [  3.95485714285 ,  10.152519999999,   0.608219026089],
                               [  3.954857142859,  12.852519999999,   0.608219026089],
                               [  5.273142857137,  10.152519999999,   0.861923230088],
                               [  5.273142857147,  12.852519999999,   0.861923230088],
                               [  1.757714285706,  10.152519999999,   1.369331638097],
                               [  1.757714285715,  12.852519999999,   1.369331638097],
                               [ -0.000000000007,   0.580519999998,   1.623035842107],
                               [  3.075999999993,   0.580519999998,   1.623035842107],
                               [ -0.000000000007,   2.524000000004,   1.623035842107],
                               [  3.075999999993,   2.524000000004,   1.623035842107],
                               [ -0.000000000007,   5.628520000005,   1.623035842107],
                               [  3.075999999993,   5.628520000005,   1.623035842107],
                               [ -0.000000000007,   7.571999999992,   1.623035842107],
                               [  3.075999999993,   7.571999999992,   1.623035842107],
                               [  3.075999999993,  10.152519999999,   1.623035842107],
                               [  3.076000000003,  12.852519999999,   1.623035842107],
                               [  5.712571428562,  10.152519999999,   2.130444250116],
                               [  5.712571428571,  12.852519999999,   2.130444250116],
                               [  0.878857142849,  10.152519999999,   2.384148454115],
                               [  0.878857142859,  12.852519999999,   2.384148454115],
                               [  1.587911227215,   9.581538781708,   2.493283401831],
                               [  4.663911227215,   9.581538781708,   2.493283401831],
                               [  1.576044222157,  -1.089252078357,   2.497495872076],
                               [  4.652044222157,  -1.089252078357,   2.497495872076],
                               [  1.537999999993,   0.            ,   2.51100055612 ],
                               [  4.613999999993,   0.            ,   2.51100055612 ],
                               [  1.537999999993,   3.104520000002,   2.51100055612 ],
                               [  4.613999999993,   3.104520000002,   2.51100055612 ],
                               [  1.537999999993,   5.048000000007,   2.51100055612 ],
                               [  4.613999999993,   5.048000000007,   2.51100055612 ],
                               [  1.537999999993,   8.152520000009,   2.51100055612 ],
                               [  4.613999999993,   8.152520000009,   2.51100055612 ],
                               [  3.515428571424,  10.152519999999,   2.891556862124],
                               [  3.515428571434,  12.852519999999,   2.891556862124],
                               [  4.833714285705,  10.152519999999,   3.145261066134],
                               [  4.833714285715,  12.852519999999,   3.145261066134],
                               [  1.31828571428 ,  10.152519999999,   3.652669474143],
                               [  1.31828571429 ,  12.852519999999,   3.652669474143],
                               [  2.636571428561,  10.152519999999,   3.906373678153],
                               [  2.636571428571,  12.852519999999,   3.906373678153],
                               [  1.537999999992,   0.580519999998,   4.286929984157],
                               [  4.613999999992,   0.580519999998,   4.286929984157],
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[1.537999999992, 2.524000000004, 4.286929984157],
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[4.613999999992, 5.628520000005, 4.286929984157],
[1.537999999992, 7.571999999992, 4.286929984157],
[4.613999999992, 7.571999999992, 4.286929984157],
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[5.273142857146, 12.852519999999, 4.413782086151],
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[0.439428571433, 12.852519999999, 4.667486290161],
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[3.075999999992, 0. , 5.17489469817],
[-0.000000000008, 3.104520000002, 5.17489469817],
[3.075999999992, 3.104520000002, 5.17489469817],
[-0.000000000008, 5.048000000007, 5.17489469817],
[3.075999999992, 5.048000000007, 5.17489469817],
[-0.000000000008, 8.152520000009, 5.17489469817],
[3.075999999992, 8.152520000009, 5.17489469817],
[3.075999999992, 10.152519999999, 5.17489469817],
[3.076000000002, 12.852519999999, 5.17489469817],
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[3.083326711623, -1.089252078357, 5.214594303051],
[0.009612107908, 9.581538781708, 5.22697766602],
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[4.394285714289, 12.852519999999, 5.42859890218],
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[0.878857142858, 12.852519999999, 5.936007310189],
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[2.197142857145, 12.852519999999, 6.189711514188],
[4.833714285704, 10.152519999999, 6.697119922197],
[4.833714285714, 12.852519999999, 6.697119922197],
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[3.075999999991, 5.628520000005, 6.950824126207],
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[2.63657142857 , 12.852519999999, 7.458232534216],
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[3.954857142857, 12.852519999999, 7.711936738215],
[1.587911227213, 9.581538781708, 7.821071685931],
[4.663911227213, 9.581538781708, 7.821071685931],
[1.576044222155, -1.089252078357, 7.825284156176],
[4.652044222155, -1.089252078357, 7.825284156176],
[1.537999999991, 0. , 7.83878884022],
[4.613999999991, 0. , 7.83878884022],

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                    [  4.613999999991,   3.104520000002,   7.83878884022 ],
                    [  1.537999999991,   5.048000000007,   7.83878884022 ],
                    [  4.613999999991,   5.048000000007,   7.83878884022 ],
                    [  1.537999999991,   8.152520000009,   7.83878884022 ],
                    [  4.613999999991,   8.152520000009,   7.83878884022 ],
                    [  0.439428571422,  10.152519999999,   8.219345146224],
                    [  0.439428571432,  12.852519999999,   8.219345146224],
                    [  1.757714285703,  10.152519999999,   8.473049350234],
                    [  1.757714285713,  12.852519999999,   8.473049350234],
                    [  4.394285714278,  10.152519999999,   8.980457758243],
                    [  4.394285714288,  12.852519999999,   8.980457758243],
                    [  5.712571428559,  10.152519999999,   9.234161962253],
                    [  5.712571428569,  12.852519999999,   9.234161962253],
                    [  1.537999999991,   0.580519999998,   9.614718268257],
                    [  4.613999999991,   0.580519999998,   9.614718268257],
                    [  1.537999999991,   2.524000000004,   9.614718268257],
                    [  4.613999999991,   2.524000000004,   9.614718268257],
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                    [  4.613999999991,   5.628520000005,   9.614718268257],
                    [  1.537999999991,   7.571999999992,   9.614718268257],
                    [  4.613999999991,   7.571999999992,   9.614718268257],
                    [  2.197142857134,  10.152519999999,   9.741570370251],
                    [  2.197142857144,  12.852519999999,   9.741570370251],
                    [  3.515428571422,  10.152519999999,   9.995274574261],
                    [  3.515428571431,  12.852519999999,   9.995274574261],
                    [ -0.00000000001 ,   0.            ,  10.50268298227 ],
                    [  3.07599999999 ,   0.            ,  10.50268298227 ],
                    [ -0.00000000001 ,   3.104520000002,  10.50268298227 ],
                    [  3.07599999999 ,   3.104520000002,  10.50268298227 ],
                    [ -0.00000000001 ,   5.048000000007,  10.50268298227 ],
                    [  3.07599999999 ,   5.048000000007,  10.50268298227 ],
                    [ -0.00000000001 ,   8.152520000009,  10.50268298227 ],
                    [  3.07599999999 ,   8.152520000009,  10.50268298227 ],
                    [ -0.00000000001 ,  10.152519999999,  10.50268298227 ],
                    [  0.            ,  12.852519999999,  10.50268298227 ],
                    [  0.007326711621,  -1.089252078357,  10.542382587151],
                    [  3.083326711621,  -1.089252078357,  10.542382587151],
                    [  3.085612107906,   9.581538781708,  10.55476595012 ]]*Angstrom

# Set up configuration
right_electrode = BulkConfiguration(
    bravais_lattice=right_electrode_lattice,
    elements=right_electrode_elements,
    cartesian_coordinates=right_electrode_coordinates
    )

# ----------------------------------------------------------
# Central region
# ----------------------------------------------------------
```

```
# Set up lattice
vector_a = [6.152, 0.0, 0.0]*Angstrom
vector_b = [0.0, 18.905, 0.0]*Angstrom
vector_c = [-9.69091473735e-12, 0.0, 31.9667297046]*Angstrom
central_region_lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
central_region_elements = [Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Silicon, Silicon, Carbon, Carbon, Silicon, Silicon, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Hydrogen,
                    Hydrogen, Hydrogen, Hydrogen, Carbon, Carbon, Silicon, Silicon,
                    Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon,
                    Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Silicon,
                    Silicon, Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Silicon,
                    Silicon, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Carbon, Hydrogen, Hydrogen,
                    Hydrogen, Hydrogen, Carbon, Carbon, Silicon, Silicon, Carbon,
                    Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Silicon,
                    Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Silicon, Silicon, Carbon, Carbon, Silicon, Silicon,
                    Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Silicon, Silicon,
                    Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen,
                    Hydrogen, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon,
                    Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Silicon,
                    Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Silicon, Silicon, Carbon, Carbon, Silicon, Silicon,
                    Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Silicon, Silicon,
                    Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen,
                    Hydrogen, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon,
                    Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Silicon,
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                    Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen,
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                    Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                    Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Silicon,
                    Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
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```

Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen, Carbon, Carbon,
Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Silicon, Silicon,
Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon,
Carbon, Carbon, Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen,
Hydrogen, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon,
Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Silicon,
Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
Carbon, Silicon, Silicon, Carbon, Carbon, Silicon, Silicon,
Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen]

Define coordinates

central_region_coordinates = [[1.318285714287, 10.152519999999, 0.10081061808],
[1.318285714287, 12.852519999999, 0.10081061808],
[3.954857142856, 10.152519999999, 0.608219026089],
[3.954857142856, 12.852519999999, 0.608219026089],
[5.273142857143, 10.152519999999, 0.861923230088],
[5.273142857143, 12.852519999999, 0.861923230088],
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[1.757714285712, 12.852519999999, 1.369331638097],
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[4.663911227221, 9.581538781708, 2.493283401831],
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[4.652044222163, -1.089252078357, 2.497495872076],
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device_configuration = DeviceConfiguration(
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# ----------------------------------------------------------------
# Calculator
# ----------------------------------------------------------------
#----------------------------------------
# Basis Set
#----------------------------------------
basis_set = [
   CerdaHuckelParameters.Silicon_GW_SiC_Basis,
   CerdaHuckelParameters.Carbon_graphite_Basis,
   CerdaHuckelParameters.Hydrogen_C2H4_Basis,
   ]

#----------------------------------------
# Numerical Accuracy Settings
#----------------------------------------
left_electrode_numerical_accuracy_parameters = NumericalAccuracyParameters(
   k_point_sampling=(10, 3, 100),
   )

right_electrode_numerical_accuracy_parameters = NumericalAccuracyParameters(
   k_point_sampling=(10, 3, 100),
   )

device_numerical_accuracy_parameters = NumericalAccuracyParameters(
   k_point_sampling=(10, 3, 100),
   )

#----------------------------------------
# Poisson Solver Settings
#----------------------------------------
left_electrode_poisson_solver = FastFourier2DSolver(
   boundary_conditions=[[PeriodicBoundaryCondition,PeriodicBoundaryCondition],
```

```
                    [PeriodicBoundaryCondition,PeriodicBoundaryCondition],
                    [PeriodicBoundaryCondition,PeriodicBoundaryCondition]]
    )

right_electrode_poisson_solver = FastFourier2DSolver(
    boundary_conditions=[[PeriodicBoundaryCondition,PeriodicBoundaryCondition],
                    [PeriodicBoundaryCondition,PeriodicBoundaryCondition],
                    [PeriodicBoundaryCondition,PeriodicBoundaryCondition]]
    )

#----------------------------------------
# Electrode Calculators
#----------------------------------------
left_electrode_calculator = HuckelCalculator(
    basis_set=basis_set,
    numerical_accuracy_parameters=left_electrode_numerical_accuracy_parameters,
    poisson_solver=left_electrode_poisson_solver,
    )

right_electrode_calculator = HuckelCalculator(
    basis_set=basis_set,
    numerical_accuracy_parameters=right_electrode_numerical_accuracy_parameters,
    poisson_solver=right_electrode_poisson_solver,
    )

#----------------------------------------
# Device Calculator
#----------------------------------------
calculator = DeviceHuckelCalculator(
    basis_set=basis_set,
    numerical_accuracy_parameters=device_numerical_accuracy_parameters,
    spin_polarization=Unpolarized,
    electrode_calculators=
        [left_electrode_calculator, right_electrode_calculator],
    )

device_configuration.setCalculator(calculator)
nlprint(device_configuration)
device_configuration.update()
nlsave('flat_structure_20.05.2016.nc', device_configuration)

# ------------------------------------------------------------
# Transmission pathways
# ------------------------------------------------------------
transmission_pathways = TransmissionPathways(
    configuration=device_configuration,
    energy=0*eV,
    kpoints=MonkhorstPackGrid(4,10),
    energy_zero_parameter=AverageFermiLevel,
    infinitesimal=1e-06*eV,
    contributions=Left,
```

```
    self_energy_calculator=DirectSelfEnergy(),
    )
nlsave('flat_structure_20.05.2016.nc', transmission_pathways)
nlprint(transmission_pathways)

# ------------------------------------------------------------
# IV curve
# ------------------------------------------------------------
biases = [0.000000, 0.066667, 0.133333, 0.200000]*Volt

iv_curve = IVCurve(
    configuration=device_configuration,
    biases=biases,
    energies=numpy.linspace(-2,2,101)*eV,
    kpoints=MonkhorstPackGrid(3,10),
    self_energy_calculator=RecursionSelfEnergy(),
    energy_zero_parameter=AverageFermiLevel,
    infinitesimal=1e-06*eV,
    selfconsistent_configurations_filename="ivcurve_selfconsistent_configurations.nc",
    )
nlsave('flat_structure_20.05.2016.nc', iv_curve)
nlprint(iv_curve)
```

Appendix C

```
# ------------------------------------------------------------
# TwoProbe configuration
# ------------------------------------------------------------

# ------------------------------------------------------------
# Left electrode
# ------------------------------------------------------------

# Set up lattice
vector_a = [18.6467807196, 0.0, 0.0]*Angstrom
vector_b = [0.0, 47.087744, 0.0]*Angstrom
vector_c = [0.0, 0.0, 5.32778828408]*Angstrom
left_electrode_lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
left_electrode_elements = [Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Silicon, Silicon,
                           Silicon, Silicon, Silicon, Silicon, Carbon, Carbon, Carbon,
                           Carbon, Carbon, Carbon, Silicon, Silicon, Carbon, Carbon, Carbon,
                           Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                           Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                           Carbon, Carbon, Carbon, Silicon, Silicon, Silicon, Silicon,
                           Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                           Silicon, Silicon, Silicon, Silicon, Silicon, Silicon, Carbon,
                           Carbon, Silicon, Silicon, Hydrogen, Hydrogen, Carbon, Carbon,
                           Carbon, Carbon, Carbon, Carbon, Silicon, Silicon, Silicon,
                           Silicon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon,
                           Carbon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                           Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                           Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Silicon,
                           Silicon, Silicon, Silicon, Silicon, Silicon, Carbon, Carbon,
                           Carbon, Carbon, Carbon, Carbon, Silicon, Silicon, Silicon,
                           Silicon, Silicon, Silicon, Carbon, Silicon, Hydrogen, Hydrogen,
                           Hydrogen, Hydrogen, Hydrogen, Hydrogen, Hydrogen, Hydrogen, Carbon,
                           Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
                           Carbon]

# Define coordinates
left_electrode_coordinates = [[  2.559770359786,  17.32465      ,   0.031624360995],
                              [  5.635770359786,  17.32465      ,   0.031624360995],
                              [  8.711770359786,  17.32465      ,   0.031624360995],
                              [ 11.787770359786,  17.32465      ,   0.031624360995],
                              [ 14.863770359786,  17.32465      ,   0.031624360995],
                              [ 17.939770359786,  17.32465      ,   0.031624360995],
                              [  2.559770359786,  20.42917      ,   0.031624360995],
                              [  5.635770359786,  20.42917      ,   0.031624360995],
                              [  8.711770359786,  20.42917      ,   0.031624360995],
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                              [ 14.863770359786,  20.42917      ,   0.031624360995],
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[8.711770359786, 22.37265 , 0.031624360995],
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[11.729855280012, 28.067670053827, 1.604661357423],
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[11.787770359786, 17.90517 , 1.807553789022],
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[4.097770359786, 20.42917 , 2.695518503036],
[7.173770359786, 20.42917 , 2.695518503036],
[10.249770359786, 20.42917 , 2.695518503036],
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[3.824091783259, 28.465444075003, 4.065663067866],
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[16.401770359786, 17.90517 , 4.471447931063],
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                    [  4.097770359786,  19.84865       ,   4.471447931063],
                    [  7.173770359786,  19.84865       ,   4.471447931063],
                    [ 10.249770359786,  19.84865       ,   4.471447931063],
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                    [  4.138069479106,  24.382188781698,   4.50581374464 ],
                    [ 13.366069479106,  24.382188781698,   4.50581374464 ],
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                    [  4.544180332819,  24.984527573138,   4.696889683368],
                    [  9.944301225157,  24.951641130803,   4.702788344818],
                    [  4.82178915042 ,  27.783983307269,   4.845581754276],
                    [  9.677751569151,  27.783983307269,   4.845581754276],
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                    [ 17.038300359786,  24.863094      ,   5.296163923087],
                    [  1.212342430467,  25.753694722212,   5.296163923087],
                    [ 13.210235527375,  26.387742443629,   5.296163923087],
                    [  2.217042171584,  26.758394463328,   5.296163923087],
                    [ 12.186510881562,  27.523449100102,   5.296163923087],
                    [  4.326441653817,  28.967793945562,   5.296163923087],
                    [ 10.09076109028 ,  29.4548558733  ,   5.296163923087],
                    [  5.83321965105 ,  29.708893590811,   5.296163923087],
                    [  8.705180359786,  29.763094      ,   5.296163923087]]*Angstrom

# Set up configuration
left_electrode = BulkConfiguration(
    bravais_lattice=left_electrode_lattice,
    elements=left_electrode_elements,
    cartesian_coordinates=left_electrode_coordinates
    )

# ----------------------------------------------------------
# Right electrode
# ----------------------------------------------------------

# Set up lattice
vector_a = [18.6467807196, 0.0, 0.0]*Angstrom
vector_b = [0.0, 47.087744, 0.0]*Angstrom
vector_c = [0.0, 0.0, 5.32778828408]*Angstrom
right_electrode_lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
right_electrode_elements = [Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
```

Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen, Hydrogen, Hydrogen,
Hydrogen, Hydrogen, Hydrogen, Hydrogen, Carbon, Carbon, Carbon,
Carbon, Carbon, Carbon, Silicon, Silicon, Silicon, Silicon,
Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
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Carbon, Carbon, Carbon, Carbon, Carbon, Silicon, Silicon, Silicon,
Silicon, Silicon, Silicon, Carbon, Carbon, Silicon, Silicon,
Hydrogen, Hydrogen, Hydrogen, Hydrogen, Carbon, Carbon, Carbon,
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Carbon, Carbon, Carbon, Carbon, Hydrogen, Hydrogen, Hydrogen,
Hydrogen, Hydrogen, Carbon, Carbon, Carbon, Carbon, Carbon,
Carbon, Carbon, Carbon, Carbon, Carbon, Silicon, Silicon, Silicon,
Silicon, Silicon, Silicon, Carbon, Carbon, Carbon, Carbon, Carbon,
Carbon, Silicon, Silicon, Silicon, Silicon, Silicon, Silicon,
Carbon, Silicon]

# Define coordinates
right_electrode_coordinates = [[15.617440359786, 24.863094 , 0.006573132836],
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[1.212342430467, 25.753694722212, 2.467574843279],
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# Set up configuration
right_electrode = BulkConfiguration(
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    elements=right_electrode_elements,
    cartesian_coordinates=right_electrode_coordinates
    )

# ------------------------------------------------------------
# Central region
# ------------------------------------------------------------

# Set up lattice
vector_a = [18.6467807196, 0.0, 0.0]*Angstrom
vector_b = [0.0, 47.087744, 0.0]*Angstrom
vector_c = [0.0, 0.0, 20.4613859161]*Angstrom
central_region_lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
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# Set up configuration
central_region = BulkConfiguration(
   bravais_lattice=central_region_lattice,
   elements=central_region_elements,
   cartesian_coordinates=central_region_coordinates
   )

device_configuration = DeviceConfiguration(
   central_region,
   [left_electrode, right_electrode]
   )

# ----------------------------------------------------------------
# Calculator
# ----------------------------------------------------------------
#----------------------------------------
# Basis Set
#----------------------------------------
basis_set = [
   CerdaHuckelParameters.Silicon_GW_SiC_Basis,
   CerdaHuckelParameters.Carbon_graphite_Basis,
   CerdaHuckelParameters.Hydrogen_C2H4_Basis,
   ]

#----------------------------------------
# Numerical Accuracy Settings
#----------------------------------------
left_electrode_numerical_accuracy_parameters = NumericalAccuracyParameters(
   k_point_sampling=(4, 4, 100),
   )

right_electrode_numerical_accuracy_parameters = NumericalAccuracyParameters(
   k_point_sampling=(4, 4, 100),
   )

device_numerical_accuracy_parameters = NumericalAccuracyParameters(
   k_point_sampling=(4, 4, 100),
   )

#----------------------------------------
# Poisson Solver Settings
#----------------------------------------
left_electrode_poisson_solver = FastFourier2DSolver(
   boundary_conditions=[[PeriodicBoundaryCondition,PeriodicBoundaryCondition],
                        [PeriodicBoundaryCondition,PeriodicBoundaryCondition],
                        [PeriodicBoundaryCondition,PeriodicBoundaryCondition]]
   )
```

```
right_electrode_poisson_solver = FastFourier2DSolver(
    boundary_conditions=[[PeriodicBoundaryCondition,PeriodicBoundaryCondition],
                         [PeriodicBoundaryCondition,PeriodicBoundaryCondition],
                         [PeriodicBoundaryCondition,PeriodicBoundaryCondition]]
    )

#----------------------------------------
# Electrode Calculators
#----------------------------------------
left_electrode_calculator = HuckelCalculator(
    basis_set=basis_set,
    numerical_accuracy_parameters=left_electrode_numerical_accuracy_parameters,
    poisson_solver=left_electrode_poisson_solver,
    )

right_electrode_calculator = HuckelCalculator(
    basis_set=basis_set,
    numerical_accuracy_parameters=right_electrode_numerical_accuracy_parameters,
    poisson_solver=right_electrode_poisson_solver,
    )

#----------------------------------------
# Device Calculator
#----------------------------------------
calculator = DeviceHuckelCalculator(
    basis_set=basis_set,
    numerical_accuracy_parameters=device_numerical_accuracy_parameters,
    spin_polarization=Unpolarized,
    electrode_calculators=
        [left_electrode_calculator, right_electrode_calculator],
    )

device_configuration.setCalculator(calculator)
nlprint(device_configuration)
device_configuration.update()
nlsave('script_for_step_structure_20.05.2017.nc', device_configuration)

# ----------------------------------------------------------------
# Transmission pathways
# ----------------------------------------------------------------
transmission_pathways = TransmissionPathways(
    configuration=device_configuration,
    energy=0.12*eV,
    kpoints=MonkhorstPackGrid(4,4),
    energy_zero_parameter=AverageFermiLevel,
    infinitesimal=1e-06*eV,
    contributions=Left,
    self_energy_calculator=DirectSelfEnergy(),
    )
nlsave('script_for_step_structure_20.05.2017.nc', transmission_pathways)
```

```
nlprint(transmission_pathways)

# ------------------------------------------------------------
# Transmission spectrum
# ------------------------------------------------------------
transmission_spectrum = TransmissionSpectrum(
    configuration=device_configuration,
    energies=numpy.linspace(0,0.12,101)*eV,
    kpoints=MonkhorstPackGrid(4,4),
    energy_zero_parameter=AverageFermiLevel,
    infinitesimal=1e-06*eV,
    self_energy_calculator=RecursionSelfEnergy(),
    )
nlsave('script_for_step_structure_20.05.2017.nc', transmission_spectrum)
nlprint(transmission_spectrum)

# ------------------------------------------------------------
# IV curve
# ------------------------------------------------------------
biases = [0.000000, 0.066667, 0.133333, 0.200000]*Volt

iv_curve = IVCurve(
    configuration=device_configuration,
    biases=biases,
    energies=numpy.linspace(-2,2,101)*eV,
    kpoints=MonkhorstPackGrid(4,4),
    self_energy_calculator=RecursionSelfEnergy(),
    energy_zero_parameter=AverageFermiLevel,
    infinitesimal=1e-06*eV,
    selfconsistent_configurations_filename="ivcurve_selfconsistent_configurations.nc",
    )
nlsave('script_for_step_structure_20.05.2017.nc', iv_curve)
nlprint(iv_curve)
```

Content of applied CD

File: Aleksei_Barulin_Thesis_2016.pdf