

# TIGHT BINDING MODEL OF AB STACKED BILAYER GRAPHENE

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## **DEDICATION**

This thesis is dedicated to my father, who taught me that the best kind of knowledge to have is that which is learned for its own sake. It is also dedicated to my mother, who taught me that even the largest task can be accomplished if it is done one step at a time.

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## ABSTRACT

AB stacked Bilayer graphene is a material of huge scientific interest due to the promise of superior electronic properties even when compared to monolayer graphene due to more  $\pi$  orbital overlaps in the x-y plane. In this research the Nearest Neighbor Tight-Binding (NNTB) model of AB stacked bilayer graphene will be developed. Using this NNTB approximation, a numerical analysis simulator that uses the Non-Equilibrium Greens Function (NEGF) equations to describe the quantum transport of the electrons in the bilayer graphene crystal is built using MATLAB. From this numerical analysis simulation, various metrics of interest such as the E-K dispersion relation, density of states (DOS) and the transmission coefficients will be obtained for each of the specified lattice width and length. Electronic properties of two variants of the bilayer graphene are investigated in this simulation, which are the zigzag edge and the armchair edge types. The program constructs a fitting device Hamiltonian for the NEGF equation from the specified type, width, and length. The NEGF simulation obtains the solution for the dispersion relation, DOS and transmission coefficient for each of the eigen energies iteratively until the solution converges to a minimum error threshold value. The DOS simulation showed there is a huge concentration of quantum states in the mid-band for the zigzag edge, and for the armchair edge the number of states is the largest at the 1st quartile-band and 3rd quartile-band region. Transmission coefficient of both zigzag and armchair edges show similar distribution throughout the energy spectrum; however, the coefficients magnitude of the zigzag edge is larger. Dispersion relation of zigzag edge showed no bandgap, though the armchair edge showed an alternating trend of semiconducting (with bandgap) from the  $3n-1$  and  $3n$  series and metallic (no bandgap) for  $3n+1$  series in agreement with contemporary research.

## ABSTRAK

Grafen dua lapis adalah bahan saintifik yang amat menarik kerana ianya mempunyai janji ciri-ciri elektronik yang lebih unggul berbanding grafen satu lapis. Topologi yang akan diterokai ialah timbunan AB grafen dua lapis. Hal ini kerana, struktur anjakan grafen satu lapis sesama sendiri memberikan lebih banyak pertindihan orbital  $\pi$  di satah x-y. Penyelidikan ini akan mengembangkan timbunan grafen dua lapis AB menggunakan paradigma ikatan ketat jiran terdekat (NNTB). Menggunakan penghampiran NNTB in suatu simulator numerical analysis yang menggunakan persamaan fungsi Greens tidak keseimbangan (NEGF) untuk memerihalkan transmisi kuantum elektron akan dibina. Simulator ini dibina menggunakan MATLAB sebagai bahasa program. Melalui simulasi numerical analysis ini, pelbagai metrik seperti hubungan dispersi E-K, ketumpatan keadaan (DOS) diterokai untuk setiap lebar and panjang. Sifat elektronik bagi dua variasi grafen dua lapis yang akan diterokai dalam simulasi ini adalah bagi hujung zigzag and hujung kerusi berlengan. Program ini akan membina Hamiltonian peranti yang sesuai untuk setiap variasi, lebar and panjang. Simulasi NEGF memberi penyelesaian untuk dispersi E-K, DOS, dan pekali transmisi untuk setiap tenaga eigen untuk setiap iterasi sehingga penyelesaian bertumpu dengan nilai ralat yang minima. Simulasi DOS menunjukkan bahawa terdapat banyak konsentrasi keadaan kuantum di jalur tengah untuk hujung zigzag, dan bagi hujung kerusi berlengan bilangan keadaan kuantum yang paling banyak adalah di kuartil 1 dan 3. Pekali transmisi bagi hujung zigzag dan kerusi berlengan menunjukkan distribusi yang sama, tapi nilai pekali bagi hujung zigzag adalah lebih besar. Dispersi E-K bagi hujung zigzag tidak mempunyai jurang band tetapi hujung kerusi berlengan menunjukan arah aliran yang berayun antara aliran yang semikonduktor dan berlogam. Keputusan ini adalah sama dengan keputusan kajian di jurnal saintifik.

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## LIST OF ABBREVIATIONS

DOS	-	Density of States
NEGF	-	Non-Equilibrium Green's Function
AGNR	-	Armchair Graphene Nanoribbon
ZGNR	-	Zigzag Graphene Nanoribbon
AGNRM	-	Monolayer Armchair Graphene Nanoribbon
ABGNR,	-	Bilayer Armchair Graphene Nanoribbon
AGNRB		
ZBGNR	-	Zigzag Bilayer Graphene Nanoribbon
ABZBGNR	-	AB stacked Zigzag Bilayer Graphene Nanoribbon
ABABGNR	-	AB stacked Armchair Bilayer Graphene Nanoribbon
DFT	-	Density Functional Theory
SZ	-	Single zeta basis set for Density Functional Theory
DZP	-	Double zeta plus polarization basis set for Density Functional Theory

## LIST OF SYMBOLS

$\psi, \varphi$	-	Wavefunction
$H$	-	Hamiltonian operator
$t$	-	Tight-binding energy parameter
$\varepsilon$	-	Self-interaction energy parameter
$I$	-	Identity matrix
$S_{AA}$	-	Overlap integral diagonal matrix element
$S_{AB}$	-	Overlap integral off-diagonal matrix element
$H_{AA}$	-	Hamiltonian matrix diagonal element
$H_{AB}$	-	Hamiltonian matrix off-diagonal element
$\gamma_0$	-	Coupling interaction between A1 – B1 or A2 – B2 lattice points wavefunctions
$\gamma_1$	-	Coupling interaction between A2 – B1 lattice points wavefunctions
$\gamma_3$	-	Coupling interaction between B2 – A1 lattice points wavefunctions
$\gamma_4$	-	Coupling interaction between A2 – A1 or B2 – B1 lattice points wavefunctions
$G^R$	-	Retarded Green's Function
$g_{s,d}^{surface}$	-	Surface Green's Function
$\tau$	-	Coupling Hamiltonian
$\dagger$	-	Matrix transpose indicator
$\lambda$	-	Wavefunction wavelength
$\nabla$	-	Del operator
$\nabla^2$	-	Laplacian operator
$\vec{r}$	-	Position vector
$\vec{p}$	-	Momentum vector
$\vec{E}$	-	Electric field vector
$\eta$	-	A very small real number $\in \mathbb{R}$
$\delta(x)$	-	The Dirac delta function

$\Gamma, \beta$	-	Contact coupling coefficient
$\delta_l$	-	Relative distance vector from local $\pi$ orbitals
$\Sigma$	-	Matrix representing wavefunction spread from channel into the contacts
$\alpha$	-	A unit cell consisting of one or more blocks strung together width wise
$\alpha_u$	-	One defined block
$\beta_w$	-	Unit cell blocks width wise coupling interactions
$\beta_l$	-	Unit cell length wise coupling interactions



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# CHAPTER 1

## INTRODUCTION

### 1.1 Introduction

Silicon based devices are found to be too slow and power hungry, hence a new novel material is proposed to overcome these hurdles, which is the AB stacked Bilayer Graphene. Monolayer Graphene has superior electronic properties and is already been extensively explored. Now the electronic transport properties of AB stacked Bilayer Graphene is explored. If AB stacked Bilayer Graphene properties are found to be exceptional, this will open the doors to faster, and less power-hungry devices to power our future.

### 1.2 Objectives

The objective of this project can be split into 3 main components, the first is to produce the equations for the  $\pi$  electron – electron interactions of the bilayer graphene unit cells and neighbouring unit cells using nearest neighbour tight binding model in the form of the Hamiltonian, alpha and beta matrices. Then these matrices are used to form the NEGF numerical method equations to build the bilayer graphene simulator to yield the dispersion relation, and other electron wave properties of bilayer graphene. Once the simulation profile is obtained the simulation results such as the dispersion relation, DOS, transmission coefficients are then benchmarked against other published observation or other simulation runs that are found in the literature as validation.

### **1.3 Research Scope**

The research is to explore the electronics properties of AB stacked bilayer graphene that emerges from this quantum systems geometric interactions of the  $\pi$  bonds of neighbouring electrons, by creating a device modelling framework via numerical analysis simulation. The smallest unit cell of the AB stacked bilayer graphene ribbons dimensions will be 3-unit cell in length (source, channel and drain) and 16 (8 top and 8 bottom layer) carbon atoms wide in a zig – zag topology. The electronic properties of interest are the E-K dispersion relation, density of states, and transmission coefficient. The device modelling framework will be formalized in the Non-Equilibrium Greens Function (NEGF) numerical method, which will be coded in MATLAB.

### **1.4 Research Contribution**

Most of the contemporary quantum simulation is done on the electron transport properties of monolayer graphene, however not much simulation research is done on bilayer graphene. Hence this project serves to develop a numerical analysis simulation framework from first principles from the ground up, starting by creating a quantum mechanical model, which is described in the NEGF numerical method and coded in a programming language of choice. This code in this project is implemented in MATLAB, because it's a powerful matrix operations tool with good visualization framework to plot the relations and simulation results. The simulator that is being developed in this project is a more cost-effective alternative to more commercial software tools such as Quantum Wise Virtual Nano Lab or Synopsys Quantum ATK albeit with lower functionality. This work will make it easier for future readers to build quantum device simulators, as the NEGF analytical method is the foundation of most of the quantum transport in device simulation engines.

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