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 π 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 NEFG 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

Grafin dua lapis adalah bahan saintific yang amat menarik kerana ianya mempunyai janji ciri-ciri electronik yang lebih unggul berbanding grafin satu lapis. Topologi yang akan diterokai ialah timbunan AB grafin dua lapis. Hal ini kerana, struktur anjakan grafin satu lapis sesama sendiri memberikan lebih banyak pertindihan orbital π di satah x-y. Penyelidikan ini akan mengembangkan timbunan grafin dua lapis AB mengunakan paradigma ikatan ketat jiran terdekat (NNTB). Mengunakan penghampiran NNTB in suatu simulator numerical analysis yang mengunakan persamaan fungsi Greens tidak keseimbangan (NEGF) untuk memerihalkan transmisi kuantum elektron akan dibina. Simulator ini dibina mengunakan MATLAB sebagai bahasa program. Melalui simulasi numerical analysis ini, pelbagai metrik seperti hubungan dispersi E-K, ketumpatan keadaan (DOS) diterokai untuk setiap lebar and panjangan. Sifat elektronik bagi dua variasi grafin dua lapis yang akan diterokai dalam simulasi ini adalah bagi hujungan zigzag and hujungan 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 hujungan zigzag, dan bagi hujungan kerusi berlengan bilangan keadaan kuantum yang paling banyak adalah di kuartil 1 dan 3. Pekali transmisi bagi hujungan zigzag dan kerusi berlengan menujukkan distribusi yang sama, tapi nilai pekali bagi hujungan zigzag adalah lebih besar. Dispersi E-K bagi hujungan zigzag tidak mempunyai jurang band tetapi hujungan kerusi berlengan menujukan 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, AGNRB	-	Bilayer Armchair Graphene Nanoribbon
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

ψ, φ	-	Wavefunction
H	-	Hamiltonian operator
t	-	Tight-binding energy parameter
ε	-	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
γ_0	-	Coupling interaction between A1 – B1 or A2 – B2 lattice points wavefunctions
γ_1	-	Coupling interaction between A2 – B1 lattice points wavefunctions
γ_3	-	Coupling interaction between B2 – A1 lattice points wavefunctions
γ_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
τ	-	Coupling Hamiltonian
†	-	Matrix transpose indicator
λ	-	Wavefunction wavelength
∇	-	Del operator
∇^2	-	Laplacian operator
$\vec{r}$	-	Position vector
$\vec{p}$	-	Momentum vector
$\vec{\vec{E}}$	-	Electric field vector
η	-	A very small real number $\in \mathbb{R}$
$\delta(x)$	-	The Dirac delta function

Γ, β	-	Contact coupling coefficient
δ_l	-	Relative distance vector from local π orbitals
Σ	-	Matrix representing wavefunction spread from channel into the contacts
α	-	A unit cell consisting of one or more blocks strung together width wise
α_u	-	One defined block
β_w	-	Unit cell blocks width wise coupling interactions
β_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 π 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 π 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.

REFERENCES

[1] S. Datta, *Electronic transport in mesoscopic systems*. Cambridge university press, 1997.

[2] C. J. Davisson and L. H. Germer, "Reflection of Electrons by a Crystal of Nickel," *Proceedings of the National Academy of Sciences of the United States of America,* vol. 14, no. 4, p. 317, 1928.

[3] N. Bohr, "I. On the constitution of atoms and molecules," *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science,* vol. 26, no. 151, pp. 1-25, 1913.

[4] E. Schrödinger, "An undulatory theory of the mechanics of atoms and molecules," *Physical review,* vol. 28, no. 6, p. 1049, 1926.

[5] T. M. MacRobert, "Spherical harmonics: an elementary treatise on harmonic functions with applications," 1947.

[6] M. Born and K. Huang, *Dynamical theory of crystal lattices*. Clarendon press, 1954.

[7] J. Garza, J. A. Nichols, and D. A. Dixon, "The Hartree product and the description of local and global quantities in atomic systems: A study within Kohn–Sham theory," *The Journal of Chemical Physics,* vol. 112, no. 3, pp. 1150-1157, 2000.

[8] D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics*. Cambridge University Press, 2018.

[9] T. Sommerfeld, "Lorentz trial function for the hydrogen atom: a simple, elegant exercise," *Journal of Chemical Education,* vol. 88, no. 11, pp. 1521-1524, 2011.

[10] S. Jenkins, "The Many Body Problem and Density Functional Theory," ed, 1997.

[11] J. C. Slater, "A simplification of the Hartree-Fock method," *Physical review,* vol. 81, no. 3, p. 385, 1951.

[12] X.-G. Zhang, K. Varga, and S. T. Pantelides, "Generalized Bloch theorem for complex periodic potentials: A powerful application to quantum transport calculations," *Physical Review B,* vol. 76, no. 3, p. 035108, 2007.

[13] R. Ram-Mohan and L. R. Ram-Mohan, *Finite element and boundary element applications in quantum mechanics*. Oxford University Press on Demand, 2002.

[14] S. Datta, *Quantum transport: atom to transistor*. Cambridge university press, 2005.

[15] N. W. Ashcroft and N. D. Mermin, "Solid state physics (saunders college, philadelphia, 1976)," *Appendix N,* vol. 166, 2010.

[16] D. A. Neamen, *Semiconductor physics and devices: basic principles*. New York, NY: McGraw-Hill, 2012.

[17] T. Li and S.-P. Lu, "Quantum conductance of graphene nanoribbons with edge defects," *Physical Review B,* vol. 77, no. 8, p. 085408, 2008.

[18] G. Liang, N. Neophytou, M. S. Lundstrom, and D. E. Nikonov, "Contact effects in graphene nanoribbon transistors," *Nano letters,* vol. 8, no. 7, pp. 1819-1824, Jul 2008, doi: 10.1021/nl080255r.

[19] V.-N. Do, "Non-equilibrium Green function method: theory and application in simulation of nanometer electronic devices," *Advances in Natural Sciences: Nanoscience and Nanotechnology,* vol. 5, no. 3, p. 033001, 2014.

[20] E. McCann and M. Koshino, "The electronic properties of bilayer graphene," *Reports on Progress in Physics,* vol. 76, no. 5, p. 056503, May 2013, doi: 10.1088/0034-4885/76/5/056503.
[21] H. Raza, *Graphene nanoelectronics: metrology, synthesis, properties and applications*. Springer Science & Business Media, 2012.
[22] C. H. Lewenkopf and E. R. Mucciolo, "The recursive Green's function method for graphene," *Journal of Computational Electronics,* vol. 12, no. 2, pp. 203-231, 2013.
[23] M. Poljak, K. Wang, and T. Suligoj, "Variability of bandgap and carrier mobility caused by edge defects in ultra-narrow graphene nanoribbons," *Solid-State Electronics,* vol. 108, pp. 67-74, 2015.
[24] M. Noei, S. M. Tabatabaei, and M. Fathipour, "Numerical analysis of ballistic ultrathin graphene nanoribbon field effect transistors," in *20th Iranian Conference on Electrical Engineering (ICEE2012)*, 2012: IEEE, pp. 255-259.
[25] D. Odili, Y. Wu, P. Childs, and D. Herbert, "Modeling charge transport in graphene nanoribbons and carbon nanotubes using a Schrödinger-Poisson solver," *Journal of Applied Physics,* vol. 106, no. 2, p. 024509, 2009.
[26] S.-K. Chin, K.-T. Lam, D. Seah, and G. Liang, "Quantum transport simulations of graphene nanoribbon devices using Dirac equation calibrated with tight-binding π-bond model," *Nanoscale research letters,* vol. 7, no. 1, pp. 1-7, 2012.
[27] S. Datta, M. Lundstrom, M. A. Alam, and J. Appenzeller, "2009 NCN@ Purdue Summer School: Electronics from the Bottom Up," 2009.
[28] P. Hawkins, M. Begliarbekov, M. Zivkovic, S. Strauf, and C. P. Search, "Quantum transport in graphene nanoribbons with realistic edges," *The Journal of Physical Chemistry C,* vol. 116, no. 34, pp. 18382-18387, 2012.
[29] C.-Z. Wang, W.-C. Lu, Y.-X. Yao, J. Li, S. Yip, and K.-M. Ho, "Tight-binding Hamiltonian from first-principles calculations," *Scientific Modeling and Simulation SMNS,* vol. 15, no. 1-3, pp. 81-95, 2008.
[30] S. Ganguly and S. Hong, "NEGF Simulation of Electron Transport in Carbon Nano-tubes and Graphene Nano-ribbons," *Purdue Nanoelectronic Computational Network (NCN),* 2009.
[31] S. Datta, "Nanoscale device modeling: the Green's function method," *Superlattices and microstructures,* vol. 28, no. 4, pp. 253-278, 2000.
[32] W. Tao, G. Qing, L. Yan, and S. Kuang, "A comparative investigation of an AB-and AA-stacked bilayer graphene sheet under an applied electric field: A density functional theory study," *Chinese Physics B,* vol. 21, no. 6, p. 067301, 2012.
[33] M. Junaid and G. Witjaksono, "Analysis of band gap in AA and Ab stacked bilayer graphene by Hamiltonian tight binding method," in *2019 IEEE International Conference on Sensors and Nanotechnology*, 2019: IEEE, pp. 1-4.
[34] J. Padilha, M. P. Lima, A. J. da Silva, and A. Fazzio, "Bilayer graphene dual-gate nanodevice: An ab initio simulation," *Physical Review B,* vol. 84, no. 11, p. 113412, 2011.
[35] M. Poljak, M. Glavan, and S. Kuzmić, "Accelerating simulation of nanodevices based on 2D materials by hybrid CPU-GPU parallel computing," in *2019 42nd International Convention on Information and Communication*

Technology, Electronics and Microelectronics (MIPRO), 2019: IEEE, pp. 47-52.
[36] N. Schlünzen, J.-P. Joost, and M. Bonitz, "Achieving the scaling limit for nonequilibrium Green functions simulations," *Physical review letters,* vol. 124, no. 7, p. 076601, Feb 21 2020, doi: 10.1103/PhysRevLett.124.076601.
[37] M. S. Hussain, "An Improved Physics Based Numerical Model of Tunnel FET Using 2D NEGF Formalism," *arXiv preprint arXiv:2003.12568,* 2020.
[38] Z. Lin *et al.*, "DFT coupled with NEGF study of structural, electronic and transport properties of two-dimensional InOBr," *Vacuum,* vol. 182, p. 109745, 2020.
[39] M. Thoss and F. Evers, "Perspective: Theory of quantum transport in molecular junctions," *The Journal of chemical physics,* vol. 148, no. 3, p. 030901, Jan 21 2018, doi: 10.1063/1.5003306.
[40] I. A. Calafell *et al.*, "Quantum computing with graphene plasmons," *npj Quantum Information,* vol. 5, no. 1, pp. 1-7, 2019.
[41] F. W. Chen, H. Ilatikhameneh, G. Klimeck, Z. Chen, and R. Rahman, "Configurable electrostatically doped high performance bilayer graphene tunnel FET," *IEEE Journal of the Electron Devices Society,* vol. 4, no. 3, pp. 124-128, 2016.
[42] Q. Zhang, J. Jiang, and K. Chan, "Electrically controllable spin transport in bilayer graphene with Rashba spin-orbit interaction," *Physics Letters A,* vol. 383, no. 24, pp. 2957-2962, 2019.
[43] A. Shokri, M. Esrafilian, and N. Salami, "Quantum transport of tunnel field effect transistors based on bilayer-graphene nanoribbon heterostructures," *Physica E: Low-dimensional Systems and Nanostructures,* vol. 119, p. 113908, 2020.
[44] M. Abdi, H. Bencherif, T. Bendib, F. Meddour, and M. Chahdi, "Significant improvement of infrared graphene nanoribbon phototransistor performance: A quantum simulation study," *Sensors and Actuators A: Physical,* vol. 317, p. 112446, 2021.
[45] A. V. Rozhkov, A. Sboychakov, A. Rakhmanov, and F. Nori, "Electronic properties of graphene-based bilayer systems," *Physics Reports,* vol. 648, pp. 1-104, 2016.
[46] S. Konschuh, M. Gmitra, D. Kochan, and J. Fabian, "Theory of spin-orbit coupling in bilayer graphene," *Physical Review B,* vol. 85, no. 11, p. 115423, 2012.
[47] A. Kuzmenko, I. Crassee, D. Van Der Marel, P. Blake, and K. Novoselov, "Determination of the gate-tunable band gap and tight-binding parameters in bilayer graphene using infrared spectroscopy," *Physical Review B,* vol. 80, no. 16, p. 165406, 2009.
[48] P. Gava, M. Lazzeri, A. M. Saitta, and F. Mauri, "Ab initio study of gap opening and screening effects in gated bilayer graphene," *Physical Review B,* vol. 79, no. 16, p. 165431, 2009.
[49] E. S. Morell, R. Vergara, M. Pacheco, L. Brey, and L. Chico, "Electronic properties of twisted bilayer nanoribbons," *Physical Review B,* vol. 89, no. 20, p. 205405, 2014.
[50] K.-T. Lam and G. Liang, "An ab initio investigation of monolayer and bilayer graphene nanoribbon based on different basis sets," 2008.

[51] K.-T. Lam and G. Liang, "An ab initio study on energy gap of bilayer graphene nanoribbons with armchair edges," *Applied Physics Letters,* vol. 92, no. 22, p. 223106, 2008.