UNIVERSITI PUTRA MALAYSIA

DENSITY FUNCTIONAL CALCULATION FOR ELECTRONIC STRUCTURE PROPERTIES OF GRAPHENE ADSORBED WITH GaAs NANOSTRUCTURE

SHAMSU ABUBAKAR

FS 2014 89

DENSITY FUNCTIONAL CALCULATION FOR ELECTRONIC STRUCTURE PROPERTIES OF GRAPHENE ADSORBED WITH GaAs NANOSTRUCTURE

By

SHAMSU ABUBAKAR

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfillment of the Requirements for the Degree of Master of Science

June 2014

DEDICATION

Dedicated to my wife and to my children, Sultan and Mama

Abstract of the thesis presented to the Senate of Universiti Putra Malaysia in fulfillment of the requirement for the degree of Master of Science

DENSITY FUNCTIONAL CALCULATION FOR ELECTRONIC STRUCTURE PROPERTIES OF GRAPHENE ADSORBED WITH GaAs NANOSTRUCTURE

By

SHAMSU ABUBAKAR

June 2014

Chairman: Md. Mahmudur Rahman, PhD

Faculty: Science

Graphene and GaAs nanostructures are well-known materials that have potential application in modern high-speed electronic devices, due to high electron mobility which makes their properties desirable. Until now, the adsorption mechanism of GaAs nanostructure on graphene with a view to change its electronic structure properties has yet to be understood. For that reason, this study is conducted on altering the electronic structure properties of graphene, as semi-metallic material using GaAs nanostructures. This semi-metallic nature needs to be overcome before graphene can be proposed as a metal-substrate for nanoscale growth.

In this work, density functional calculation employed is based on quantum mechanical method, used to examine the possible effect of small number of adsorbed Ga and As adatoms as well as their dimer on graphene. This calculation is performed using exchange-correction functional to obtain the structural stabilities and electronic properties of graphene adsorbed with GaAs nanostructure. A simplifying approach of *k*-points sampling and pseudopotentials approximation are also used in the calculation. The computational software package used based on density functional theory for this calculation is QUANTUM ESPRESSO.

The results of the calculation have indicated that the convergences with respect to plane-wave energy cutoff and with *k*-points sampling grids have been achieved. This calculation is performed in order to determine the stable height between the Ga and As adatoms on graphene and subsequently, the most stable adsorption sites of the individual atoms and dimer on graphene are obtained. After optimization, the lattice constant for a pristine graphene, a = 2.46 Å is in agreements with the experimental value found in literatures. For the calculated adsorption site of Ga adatom on graphene, H-site is found to be energetically stable. The bond distance between gallium adatom and the neighboring carbon atoms in the graphene structure on H-site is 2.26Å, which is in closer agreement with the value of 2.20Å, found in other previous study. In the case of arsenic adatom on graphene, B-site is the most stable adsorption site and the electronic structure of graphene is affected significantly, as a result of the charge transfer and weak hybridization.

The magnetic moment for gallium and arsenic adatoms as well as their dimer is found to be 0.00, which signify the non-magnetic behavior in graphene that is adsorbed with GaAs nanostructure. It has also been found that the orbital contributions for C-GaAs bond are mainly dominated by p_z orbitals of carbon and p_x and p_y orbitals of GaAs.

This study has significantly found that the semi-metallic behavior in graphene is changed to metallic as a result of orbitals-hybridization with GaAs nanostructure. Therefore, these new features make graphene a wonderful material for potential uses in electronic device and also as prepared substrate, used for the epitaxial growth of nanowires.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Master Sains

PENGIRAAN FUNGSI KETUMPATAN UNTUK SIFAT STRUKTUR ELEKTRONIK BAGI GRAFEN TERJERAP DENGAN STRUKTUR NANO GaAs

Oleh

SHAMSU ABUBAKAR

Jun 2014

Pengerusi: Md. Mahmudur Rahman, PhD

Fakulti: Sains

Grafen dan strukturnano GaAs adalah bahan yang terkenal yang mempunyai aplikasi yang berpotensi dalam peranti kelajuan tinggi moden elektronik, kerana mobiliti elektron tinggi yang menjadikan sifat mereka diperlukan. Sehingga kini, mekanisme punjerapan struktur nano GaAs pada grafen dengan tujuan untuk mengubah sifat struktur elektronik masih belum difahami. Atas sebab itu, kajian ini dijalankan ke atas mengubah sifat-sifat struktur elektronik grafen, sebagai bahan separa-logam menggunakan strukturnano. Sifat separa logam perlu diatasi sebelum grafen boleh dicadangkan sebagai logam-substrat untuk pertumbuhan skala nano.

Dalam penyelidikan ini, pengiraan fungsi ketumpatan digunakan adalah berdasarkan kaedah mekanik kuantum, digunakan untuk memeriksa kesan kemungkinan sebilangan kecil terjerap adatom Ga dan As serta dimer mereka pada grafen. Pengiraan ini dilakukan dengan menggunakan pertukaran pembetulan berfungsi untuk mendapatkan kestabilan struktur dan sifat-sifat elektronik grafen terjerap dengan struktur nano GaAs. Pendekatan mudahtitik-k persampelan dan anggaran keupayaan psuedo juga digunakan dalam pengiraan. Pakej perisian pengiraan yang digunakan berdasarkan teori fungsi ketumpatan untuk pengiraan ini adalah “QUANTUMESPRESSO”.

Keputusan pengiraan telah menunjukkn bahawa pencapahanterhadap tenaga satah-gelombeng penggal dan dengan grid titik-k persampelan telah tercapai. Pengiraan ini dilakukan untuk menentukan ketinggian yang stabil antara adatom Ga dan As pada grafen dan seterusnya, tapak penjerapan yang paling stabil daripada atom individu dan dimer pada grafen diperolehi. Selepas pengoptimuman, pemalar kekisi untuk grafen bersih, a = 2.46 Å adalah sama dengan nilai ujikaji yang terdapat dalam literatur. Untuk tapak penjerapan yang dikira adatom Ga pada grafen, tapak-Hdidapati amat stabil. Jarak ikatan antara adatom galium dan atom karbon jiran dalam struktur grafen pada tapak-Hadalah 2.26Å, yang berada dalam nilai lebih dekat dengan nilai 2.20Å, ditemui dalam kajian yang terdahulu. Dalam kes adatom arsenik pada grafen, tapak-B adalah tapak penjerapan yang paling stabil dan struktur elektronik grafen terjejas dengan ketara, akibat daripada pemindahan cas dan penghibridan lemah.

Momen magnetuntuk adatom galium dan arsenik serta dimer didapati 0.00, yang menandakan tingkah laku bukan magnet dalam grafen yang terjerap dengan strukturnanoGaAs. Ia juga telah mendapati bahawa sumbangan orbit untuk ikatan C-GaAs kebanyakannya dikuasai oleh orbital p_z karbon dan p_x dan orbital p_y daripada GaAs.

Kajian ini telah mendapati bahawa dengan ketara tingkah laku separa logam dalam grafen ditukar kepada logam akibat daripada orbital-penghibridan dengan strukturnanoGaAs. Oleh itu, ciri-ciri ini baru membuat grafen sebagai bahan yang menarik untuk digunakan dan berpotensi dalam peranti elektronik dan juga substrat seperti yang disediakan, digunakan untuk pertumbuhan permukaan wayar nano.

ACKNOWLEDGEMENTS

All praise is to Allah for the successful completion of my Master program. I would like to extend my sincere gratitude to my supervisor, Dr. Md. Mahmudur Rahman, for his invaluable guidance and support throughout my candidature. His scholarly criticisms, scrutiny, patience and suggestions are the main ingredients of my success. In addition, I would like to thank Assoc. Prof. Dr. Hishamuddin Zainuddin for his role as my co-supervisor; his rapid replies and wonderful comments indeed made me a better research student.

This research journey would not have been successful without the immense moral support of my family, my mother, Hajiya Habiba and my father Alhaji Abubakar Tambaya. I would like to specially thank my wife, Hadiza, for her loyalty, love, patience, emotional support and enduring trials that we have gone together during her stay in Malaysia and also my children, Sultan and Mama. I would like to thank my brothers and sister, Ibrahim Abubakar, Lawal Abubakar and Zainab Abubakar, who took care of some of my responsibilities diligently, while I was away for good two years. Appreciation also goes to our elder brother and all his family members; Alhaji Sani Badamasi, who supported me financially and morally. I would never forget to mention my active fellow research group member Yusuf Zuntu Abdullahi and friends Sultan Maiyaki, Alhasan Shuaibu, Sani Jibrin; for their support, friendly advice and whose efforts constructs a nice bridge for me to manage my research journey and kept going against all odds. I wish to thank the Nigerian community in UPM, being an umbrella for us to share our feeling socially and academically.

Finally, special thanks to all and sundry who in one way or the other helped me to achieve my goal, whose name I failed to mention due to my own limitations.
I thank you all.

I certify that a Thesis Examination Committee has met on 16 June 2014 to conduct the final examination of Shamsu Abubakar on his thesis entitled "Density Functional Calculation for Electronic Structure Properties of Graphene Adsorbed with GaAs nanostructure" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Master of Science.

Members of the Thesis Examination Committee were as follows:

Zainal Abidin b Talib, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Zaidan b Abdul Wahab, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Lim Kean Pah, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Sib Krishna Ghoshal, PhD
Associate Professor
Universiti Technology Malaysia
(External Examiner)

NORITAH OMAR, PhD
Professor and Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date:

This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfillment of the requirement for the degree of Master of Science. The members of the Supervisory Committee were as follows:

Md. Mahmudur Rahman, PhD
Senior Lecturer
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Hishamuddin b Zainuddin, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

BUJANG BIN KIM HUAT, PhD
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date:

Declaration by graduate student

I hereby confirm that:

- this thesis is my original work;
- quotations, illustrations and citations have been duly referenced;
- this thesis has not been submitted previously or concurrently for any other degree at-any other institutions;
- Intellectual property from thesis and copyright of thesis are fully owned by Universiti Putra Malaysia, as according to the Universiti Putra Malaysia (Research) Rules 2012;
- Written permission must be obtained from supervisor and the office of Deputy Vice-Chancellor (Research and Innovation) before thesis is published (in the form of written, printed or in electronic form) including books, journals, modules, proceedings, popular writings, seminar papers, manuscripts, posters, reports, lecture notes, learning modules or any other materials as stated in the Universiti Putra Malaysia (Research) Rules 2012;
- there is no plagiarism or data falsification/fabrication in the thesis, and scholarly Integrity is upheld as according to the Universiti Putra Malaysia (Graduate Studies) Rules 2003 (Revision 2012-2013) and the Universiti Putra Malaysia (Research) Rules 2012. The thesis has undergone plagiarism detection software.

Signature:_____ Date: _____

Name and Matric No.**:** _____

Declaration by Members of Supervisory Committee

This is to confirm that:

- The research conducted and the writing of this thesis was under our supervision;
- Supervision responsibilities as stated in Rule 41 in Rules 2003 (Revision 2012–2013) were adhered to.

Signature: _____	Signature: _____
Name of Chairman of Supervisory Committee:	Name of Member of Supervisory Committee:

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

ABINIT	Abnitio Simulation package
AE	All-electron
BOA	Born-Oppenheimer Approximation
BZ	Brillouin Zone
C	Carbon
DFT	Density Functional Theory
DOS	Density of States
Ecut	Energy cut-off
E_F	Energy or Fermi energy
eV	Electron Volt
GGA	Generalized Gradient Approximation
GaAs	Gallium Arsenide
HK	Hohenberg and Kohn
HOMO	Highest Occupied Molecular Orbital
KS	Kohn and Sham
LAPW	Linearized Augmented Plane Wave
LDA	Local Density Approximation
LUMO	Lowest Unoccupied Molecular Orbital
PAW	Projector Augmented Wave
PES	Potential Energy Surface
PLD	Pulsed Laser Deposition
PW91	Perdew Wang 91
PsP	Pseudopotentials
PDOS	Projected Density of States
PW	Plane-waves
SCF	Self-Consistent Field
SIESTA	Spanish Initiative for Electronic Simulations with Thousands of Atoms
USPsP	Ultra-soft Pseudopotentials
VASP	Vienna Ab-initio Simulation Package

CHAPTER 1

INTRODUCTION

1.1 Background of the Study

The emerging needs for low-cost and efficient high-speed semiconductor devices have generated interest and motivated researchers to build different nanostructures on a very transparent, electrically conductive and flexible material for potential applications in nanoscale devices for the future use. A two-dimensional material called "Graphene" (Geim and Novoselov, 2007), is an excellent platform which serves as a substrate for nanoscale growth for development and integration of many modern electronic semiconductor devices. In this regards, new experimental and theoretical studies on the growth of various nanostructures on graphene have been reported, which includes: GaAs, GaN, and ZnO (Munshi *et al*., 2012; Ishii, Tatani, and Nakada, 2011; Lee *et al*., 2012;). However, because of the unique electronic and optical properties, quasi-one-dimensional III/V semiconducting nanostructures have enormous influence when built on a substrate, making them promising for various device applications. Presently, with the help of developed density functional theory (DFT) based computer codes (Giannozzi *et al*., 2009), available in Grids and other computer platforms for modeling and simulations, progress has been made towards understanding, modifying and controlling the electronic behavior and other properties of graphene, its surface and interfaces.

On the other hand, the miniaturization of nanoscale electronic devices, such as field-effect transistors (FETs) (Tang, Li, Chi, and Chen, 2012), have caused an urgent demand for the new theoretical findings and practical method for dealing with quantum mechanical effect in those devices(Chen and Wei, 2010).

Density functional study of the electronic and structural properties of graphene is rapidly growing field in condensed matter. A modern computational method based on density functional calculation (Kohn and Sham, 1965), has significantly contributed in the field of material science and its used to calculate the ground-state electronic properties of crystalline solids, liquids and surfaces. Simulation of such variety of materials that can be considered as an assembly of many electrons and nuclei is possible through application of density functional calculations, at the expense of one's computer memory, space and speed. In principle, density functional calculation (Martin, 2004), has become an effective way of accurately predicting useful ground-state properties of graphene, GaAs and other materials with different dimension. Therefore, the great need to improve on the computational aspect arises from the fundamental importance, practical applicability and intellectual challenges.

In the year 2004,(Novoselov *et al.,* 2004),have succeeded in isolating a single layer of graphite. In their published article, they explained the fabrication procedure and atomic force microscopy (AFM) characterization of graphene. They used a simple and effective mechanical exfoliation method for extracting thin layers of graphite from a graphite crystal with Scotch Tape and then transferred these layers to a silicon substrate. From the scientific point of view, they provide some useful properties predicted for graphene, long time ago by (Wallace, 1947).

However, the study of adsorption of atoms, molecules and clusters on graphene surfaces with a view to alter or modify its novel properties, has been a subject of discussion among researchers (Alzahrani, 2011; Mao, Yuan, and Zhong, 2008; Nakada and Ishii, 2011). In particular, due to the fact that materials are composed of nuclei bound together by electrons, higher electron mobility is an important property found in graphene, which indicates the mobile character of charge particles.

The experimental reports on the electron mobility of graphene at room temperature is approximately 15,000 $cm^2/V^{-1}sec^{-1}$, which is higher than ~1400 $cm^2/V^{-1}sec^{-1}$, the electron mobility of silicon or typical semiconductor material, and yet unsurpassed with 8500 $cm^2/V^{-1}sec^{-1}$, the mobility of Gallium Arsenide (GaAs), which is a semiconducting compound, well known for its high electron mobility (Iyechika, 2010). Graphene has emerged at the most demanding period of time, and several researches on graphene's electronic, structural and magnetic properties are still ongoing, both in theoretical and experimental sciences based on new ideas, techniques and models with a view to explore more of its exotic nature. A breakthrough in graphene science provides a fertile basis and established a platform for studying and predicting the nature of other two-dimensional system at atomic level (Aufray *et al*., 2010; Lalmi *et al.*, 2010).

1.2 Problem Statement

Being an alternative to silicon based electronics, graphene and GaAs if perfectly grown together are two important materials that have potential uses in semiconductor devices because of the high electron mobility which makes their properties functional. Despite this great achievement regarding advantages of graphene with GaAs, one big problem observed in a graphene, is the linear dispersion of energy between the valence band and the conduction band at Fermi-level, showing zero band gap semi-metallic nature (Geim and Novoselov, 2007). This semi-metallic nature needs to be overcome before graphene can be proposed as a metal-substrate, which also served as channel material for nanoscale growth.

Further effort to overcome the zero band gap nature of graphene is proposed: The band gap can be induced in graphene, either through doping or adsorption of atoms or molecules on its surface (Chan, Neaton, and Cohen, 2008; Nakada and Ishii, 2011). Thus, one of the rising fields related to graphene research is how to build nanostructures on graphene surface. Therefore, the idea of chosen GaAs nanostructure on graphene has a very interesting topical advantage that needs additional study both from theoretical and experimental part.

Until now, the adsorption mechanism of GaAs nanostructure on graphene with a view to change its electronic structure properties has yet to be understood. In this work, the effect of having a small number of adsorbed Ga and As adatoms as well as their dimer on graphene has been reported. The idea is to examine the quantum mechanical effects in graphene due to adsorption consequences of single Ga and As adatoms and GaAs dimer, using density functional calculation. It is expected that, proper adsorption of GaAs nanostructure on graphene will have a significant impact towards changing the electronic states of graphene from semi-metallic to metallic material.

However, in view of these, the following hypothetical research questions emerged:

1. Does the adsorption of a single Ga and As adatoms or dimer cause any changes on the structure and electronic properties of graphene sheet?

2. What are the binding sites for a newly adsorbed Ga and As adatoms or dimer on graphene?

3. Does the adsorption of Ga and As adatoms or dimer subsequently, change or alter the energy state of graphene?

4. How does charge transfer between Ga and As adatoms or dimer on graphene occur?

1.3 The objective of the Study

(a) To determine the structural and electronic characteristics of graphene due to Ga and As adatoms and dimer adsorption.

(b) To examine the effect of altering the electronic state of graphene by adsorption of vertically oriented GaAs dimer, for potential applications in electronics.

(c) To examine the mechanism of charge transfer between the Ga and As adatoms and dimer to graphene.

1.4 The significance of the study

Both graphene and GaAs have shown great deal in terms of properties mostly needed in electronic devices as a result of the intrinsic nature of their electrons. What really matters is the inspiration towards achieving a specific goal. For instance, potential usage of graphene as hydrogen storage media and magnetic graphene nanostructures for possible uses in spintronics has been reported. Apparently, since graphene is two-dimensional in nature, and GaAs nanostructure (dimer) is just a one-dimensional material, it's expected that the binding between graphene surface and the grown GaAs is capable to produce a good substrate material for nanoscale growth. However, the lattice mismatch between graphene and the grown GaAs nanostructure is found to be minimal, because of the flat surface nature of graphene. Therefore, the importance of these two materials (graphene and GaAs), may arises if epitaxial growth technique is employed for nanowires growth.

The Hypothesis:

The atomic structure of GaAs (adatom or dimer) has chemisorbed on graphene surface. In this case, an interesting hybridization and charge transfer occur either from graphene to GaAs or vice-versa. However, the electronic structure of graphene is expected to be changed and yields some new properties more or less, in the bands and density of states as a result of GaAs adsorption.

1.5 The scope of the study

Graphite, being a stacking layer of graphene is a good example of a material with van der Waals interaction, holding the individual layers together. Therefore, describing these interactions with density functional calculation is very challenging. In this case, restriction is on a surface of single graphene layer, raised up with about ~17Å interlayer distances, so that the interactions between the subsequent graphene layers would be negligible.

This density functional calculation is limited on adsorption properties of graphene with small number of Ga and As adatom and dimer on graphene surface. After considering

the contributions of the individual Ga and As adatoms, the small range GaAs dimer is used for the vertical configurations with a view to check its polarity on graphene. The changes in graphene electronic and structural properties which resulted from adsorption depend strongly on the type of bonds formed between carbon in the graphene structure and the GaAs nanostructure particularly, on the most favored sites. In order to achieve the objectives, only favored adsorption sites are considered for further post-processing. Moreover, the study would not attempt to examine or give an account of the magnetic exchange interaction between graphene and GaAs nanostructure, as well as the vander-Waals interactions. Therefore, only magnetic moment per unit cell of the system has been examined.

Outline of the thesis

The first chapter of this work serves as general introduction. It provides descriptions of the origin of graphene, its properties and brief area of applications, as well as short outline of the proposed method. The main aims and objectives of this research, statement of the problem, significance of the study, the hypothesis and delimitations are also arranged in this chapter.

The second chapter, reviews the relevant literature on graphene as carbon allotrope and graphene with nanomaterial (atoms and molecules), including experimental and theoretical work, are all presented. Emphasis is mainly on graphene structural characteristics.

The third chapter reflects on the theoretical foundations of the research. Electronic structure methods, solving many body problems by using electron density based method, rather than the wavefunction based. Periodic system calculations, using density functional theory within the generalized gradient approximation (GGA) are discussed.

Tight-binding model, plane-waves, self-consistent formalism, atomic pseudopotentials and how they are related to DFT and Quantum Espresso code are highlighted. Also, in this chapter, the model of our calculations, such as the constructed graphene supercells with different configurations, including the most favorable arrangements are discussed.

The fourth chapter is devoted to the discussion of the results of the calculations, as well as the new findings relevant to the data obtain. The relaxed (optimized structure), band structure and density of states (DOS) graphs are also depicted.

In the fifth chapter, the conclusions drawn from this work are given along with explanations, and finally, several ways to expand this work in future are stated together with some recommendations.

REFERENCES

Akturk et. al. (2010). Effects of silicon and germanium adsorbed on graphene. *Applied Physics Letters*, *96*(12), 123112–123113.

Alzahrani, A. Z. (2011). Structural and Electronic Properties of Graphene upon Molecular Adsorption: DFT Comparative Analysis.

Aufray, B., Kara, A., Vizzini, S., Oughaddou, H., L. andri, C., Ealet, B., & Le Lay, G. (2010). Graphene-like silicon nanoribbons on Ag (110): A possible formation of silicene. *Applied Physics Letters*, *96*(18), 183102–183103.

Bao, X.-Y., Soci, C., Susac, D., Bratvold, J., Aplin, D. P. R., Wei, W., Wang, D. (2008). Heteroepitaxial growth of vertical GaAs nanowires on Si (111) substrates by metal organic chemical vapor deposition. *Nano Letters*, *8*(11), 3755–3760.

Bonaccorso, F., Sun, Z., Hasan, T., & Ferrari, A. C. (2010). Graphene photonics and optoelectronics. *Nature Photonics*, *4*(9), 611–622.

Boukhvalov, D. W., & Katsnelson, M. I. (2008). Chemical functionalization of graphene with defects. *Nano Letters*, *8*(12), 4373–4379.

Bowman, G. (2007). *Essential quantum mechanics*. (pp1-127, Ed.) (p. 203 pages). Oxford University Press.

Cahangirov, S., & Ciraci, S. (2009). First-principles study of GaAs nanowires. *Physical Review B*, *79*(16), 165118.

Carter, V. C. and E. A. (2007). Introduction to Solid State Physics, Band Structure Theory and Periodic Density-Functional Theory.

Chan, K. T., Neaton, J. B., & Cohen, M. L. (2008). First-principles study of metal adatom adsorption on graphene. *Physical Review B*, *77*(23), 235430.

Chen, D., & Wei, G.-W. (2010). Modeling and simulation of electronic structure, material interface and random doping in nano-electronic devices. *Journal of Computational Physics*, *229*(12), 4431–4460.

Chow, P. P. (1991). Molecular beam epitaxy. *Academic Press, Inc., Thin Film Processes II(USA), 1991*, 133–175.

De Heer, W. A., Berger, C., Wu, X., First, P. N., Conrad, E. H., Li, X., Sadowski, M. L. (2007). Epitaxial graphene. *Solid State Communications*, *143*(1), 92–100.

Dreizler, R. M., & Gross, E. K. U. (1990). *Density functional theory: an approach to the quantum many-body problem* (Vol. 184). Springer-Verlag Berlin.

Emtsev, K. V, Speck, F., Seyller, T., Ley, L., & Riley, J. D. (2008). Interaction, growth, and ordering of epitaxial graphene on SiC {0001} surfaces: A comparative photoelectron spectroscopy study. *Physical Review B*, *77*(15), 155303.

Electronic structure methods: *http://en.wikipedia.org/Wiki/Electron_Configuration*.

Foldy, L. L., & Wouthuysen, S. A. (1950). On the Dirac theory of spin $^1/_2$ particles and its non-relativistic limit. *Physical Review*, *78*(1), 29.

Friedemann, M., Pierz, K., Stosch, R., & Ahlers, F. J. (2009). Graphene on gallium arsenide: Engineering the visibility. *Applied Physics Letters*, *95*(10), 102103.

Fuchs, J.-N., & Goerbig, M. O. (2008). Introduction to the physical properties of graphene. *Lecture Notes*.

Geim, A. K., & Novoselov, K. S. (2007a). The rise of graphene. *Nature Materials*, *6*(3), 183–191.

Geim, A. K., & Novoselov, K. S. (2007b). The rise of graphene. *Nature Materials*, *6*(3), 183–191.

Giannozzi, P., Baroni, S., Bonini, N., Calandra, M., Car, R., Cavazzoni, C., Dabo, I. (2009). QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics: Condensed Matter*, *21*(39), 395502.

Heiskanen, H. P., Manninen, M., & Akola, J. (2008). Electronic structure of triangular, hexagonal and round graphene flakes near the Fermi level. *New Journal of Physics*, *10*(10), 103015.

Hohenberg, P., & Kohn, W. (1964). Inhomogeneous electron gas. *Physical Review*, *136*(3B), B864.

Hu, C. H., Zheng, Y., Zhang, Y., Wu, S. Q., Wen, Y. H., & Zhu, Z. Z. (2011). Electronic and magnetic properties of silicon adsorption on graphene. *Solid State Communications*, *151*(17), 1128–1130.

Hu, L., Hu, X., Wu, X., Du, C., Dai, Y., & Deng, J. (2010). Density functional calculation of transition metal adatom adsorption on graphene. *Physica B: Condensed Matter*, *405*(16), 3337–3341.

Ishii, A., Tatani, T., & Nakada, K. (2011). Density functional calculation for growth of GaN on graphite as 3D growth on 2D material. *Physica Status Solidi (c)*, *8*(5), 1585–1588.

Iyechika, Y. (2010). Application of Graphene to High-Speed Transistors: Expectations and Challenges. *Science and Technology Trends*, *37*, 76–92.

Jiang, Z., Zhang, Y., Tan, Y.-W., Stormer, H. L., & Kim, P. (2007). Quantum Hall effect in graphene. *Solid State Communications*, *143*(1), 14–19.

Joyce, H. J., Wong-Leung, J., Gao, Q., Tan, H. H., & Jagadish, C. (2010). Phase perfection in zinc blende and wurtzite III− V nanowires using basic growth parameters. *Nano letters*, *10*(3), 908-915.

Kendall, R. A., AprÃ, E., Bernholdt, D. E., Bylaska, E. J., Dupuis, M., Fann, G. I., … Nieplocha, J. (2000). High performance computational chemistry: An overview of NWChem a distributed parallel application. *Computer Physics Communications*, *128*(1), 260–283.

Khomyakov, P. A., Giovannetti, G., Rusu, P. C., Brocks, G., Van den Brink, J., & Kelly, P. J. (2009). First-principles study of the interaction and charge transfer between graphene and metals. *Physical Review B*, *79*(19), 195425.

Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*(4A), A1133.

Kresse, G. (1996). Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Physical Review B*, *54*(16), 11169.

Kuila, T., Bose, S., Mishra, A. K., Khanra, P., Kim, N. H., & Lee, J. H. (2012). Chemical functionalization of graphene and its applications. *Progress in Materials Science*, *57*(7), 1061–1105.

Lalmi, B., Oughaddou, H., Enriquez, H., Kara, A., Vizzini, S. bastien, Ealet, B. nidicte, & Aufray, B. (2010). Epitaxial growth of a silicene sheet. *Applied Physics Letters*, *97*(22), 223102–223109.

Lavoisier, A. L. (1965). *Elements of chemistry: in a new systematic order, containing all the modern discoveries*. DoverPublications. com.

Lee, K. Y., Kumar, B., Park, H.-K., Choi, W. M., Choi, J.-Y., & Kim, S.-W. (2012). Growth of High Quality ZnO Nanowires on Graphene. *Journal of Nanoscience and Nanotechnology*, *12*(2), 1551–1554.

Leenaerts, O., Partoens, B., & Peeters, F. M. (2008). Adsorption of H2O, NH3, CO, NO2, and NO on graphene: A first-principles study. *Physical Review B*, *77*(12), 125416.

Lewars, E. (2003). *Computational chemistry*. *pp. 385-389*. Springer.

Liao, L., Lin, Y.-C., Bao, M., Cheng, R., Bai, J., Liu, Y., Duan, X. (2010). High-speed graphene transistors with a self-aligned nanowire gate. *Nature*, *467*(7313), 305-308.

Liu, X., Wang, C. Z., Yao, Y. X., Lu, W. C., Hupalo, M., Tringides, M. C., & Ho, K. M. (2011). Bonding and charge transfer by metal adatom adsorption on graphene. *Physical Review B*, *83*(23), 235411.

Mao, Y., Yuan, J., & Zhong, J. (2008). Density functional calculation of transition metal adatom adsorption on graphene. *Journal of Physics: Condensed Matter*, *20*(11), 115209.

Martin, R. M. (2004). *Electronic structure: basic theory and practical methods*. Cambridge university press.

Mattana, G. (2011). Realisation and Characterisation of Organic Electronic Devices for E-textiles applications.

Mirzadeh, M., & Farjam, M. (2012). First-principles study of bandgap effects in graphene due to hydrogen adsorption. *Journal of Physics: Condensed Matter*, *24*(23), 235304.

Mohseni, P. K., Behnam, A., Wood, J. D., English, C. D., Lyding, J. W., Pop, E., & Li, X. (2013). InGaAs Nanowire Growth on Graphene: van der Waals Epitaxy Induced Phase Segregation. *Nano Letters*, *13*(3), 1153–1161.

Monkhorst, H. J., & Pack, J. D. (1976). Special points for Brillouin-zone integrations. *Physical Review B*, *13*(12), 5188–5192.

Mukherjee, S., & Kaloni, T. P. (2012). Electronic properties of boron-and nitrogen-doped graphene: a first principles study. *Journal of Nanoparticle Research*, *14*(8), 1–5.

Munshi, A. M., Dheeraj, D. L., Fauske, V. T., Kim, D.-C., van Helvoort, A. T. J., Fimland, B.-O., & Weman, H. (2012). Vertically aligned GaAs nanowires on graphite and few-layer graphene: generic model and epitaxial growth. *Nano Letters*, *12*(9), 4570–4576.

Nakada, K., & Ishii, A. (2011). DFT Calculation for Adatom Adsorption on Graphene. *Graphene Simulation, Open Access Book Edited by Jian Ru Gong, ISBN*, 953–978.

Neckel, A., Rastl, P., Eibler, R., Weinberger, P., & Schwarz, K. (1975). Results of self-consistent band-structure calculations for ScN, ScO, TiC, TiN, TiO, VC, VN and VO. *Journal of Physics C: Solid State Physics*, *9*(4), 579.

Neto, A. H. C., Guinea, F., Peres, N. M. R., Novoselov, K. S., & Geim, A. K. (2009). The electronic properties of graphene. *Reviews of Modern Physics*, *81*(1), 109.

Novoselov, K. S., Geim, A. K., Morozov, S. V, Jiang, D., Zhang, Y., Dubonos, S. V, … Firsov, A. A. (2004). Electric field effect in atomically thin carbon films. *Science*, *306*(5696), 666–669.

Novoselov, S. (2010). The Nobel Prize in Physics 2010 honours two scientists, who have made the decisive contributions to this development. They are Andre K. Geim and Konstantin S. Novoselov, both at the University of Manchester, UK. They have succeeded in producing, isolating, identifying and characterizing graphene.

Parr, R. G., & Yang, W. (1989). *Density-functional theory of atoms and molecules* (Vol. 16). Oxford university press.

Perdew, J.P., & Zunger, A. (1981). Self-interaction correction to density-functional approximations for many-electron systems. *Physical Review B*, *23*(10), 5048.

Plachinda, P. (2012). *Electronic Properties and Structure of Functionalized Graphene, PhD Thesis, Portland State University*. *Notes*.

PPT (Ed.). (2012). Structure and Bonding in Organic Chemistry - La Salle University. Retrieved 8 August 2013 from. *www.lasalle.edu/StructureBonding.ppt*.

Rao, C. emsp14N emsp14R, Sood, A. emsp14K, Subrahmanyam, K. emsp14S, & Govindaraj, A. (2009). Graphene: The New Two Dimensional Nanomaterial. *Angewandte Chemie International Edition*, *48*(42), 7752–7777.

Reciprocal Space and Brillouin Zones in Two and Three Dimensions
https://www.chem.tamu.edu/rgroup/hughbanks/.../translation_groups3.p

Rohrl, J., Hundhausen, M., Emtsev, K. V, Seyller, T., Graupner, R., & Ley, L. (2008). Raman spectra of epitaxial graphene on SiC (0001). *Applied Physics Letters*, *92*(20), 201913–201918.

Roos, B. O. (1987). The Complete Active Space Selfâ€ • Consistent Field Method and its Applications in Electronic Structure Calculations. *Advances in Chemical Physics: Ab Initio Methods in Quantum Chemistry Part 2, Volume 69*, 399–445.

Santos, E. J. G., Ayuela, A., & Sanchez-Portal, D. (2010). First-principles study of substitutional metal impurities in graphene: structural, electronic and magnetic properties. *New Journal of Physics*, *12*(5), 53012.

Sarma, S. Das, Adam, S., Hwang, E. H., & Rossi, E. (2005). Electronic transport in two-dimensional graphene. *Reviews of Modern Physiopcs*, *83*(2), 407.

Schmidt, M. W., Baldridge, K. K., Boatz, J. A., Elbert, S. T., Gordon, M. S., Jensen, J. H., Su, S. (1993). General atomic and molecular electronic structure system. *Journal of Computational Chemistry*, *14*(11), 1347–1363.

Schwabl, F. (2005). *Advanced quantum mechanics*. Springerverlag Berlin Heidelberg.

Schwinger, J. (1948). On quantum-electrodynamics and the magnetic moment of the electron. *Physical Review*, *73*(4), 416–417.

Sholl, D., & Steckel, J. A. (2009). *Density functional theory: a practical introduction* (p. pp 233). Wiley. com.

Tang, C. L. (2005). *Fundamentals of quantum mechanics: for solid state electronics and optics* (pp. pp.1–208). Cambridge University Press.

Tang, C.-C., Li, M.-Y., Li, L. J., Chi, C. C., & Chen, J.-C. (2012). Graphene-GaAs/AlxGa1− xAs heterostructure dual-function field-effect transistor. *Applied Physics Letters*, *101*, 202104.

Trindle, C., & Shillady, D. (2008). *Electronic structure modeling: connections between theory and software* (p. pp.1–484). CRC Press.

Valencia, F., Romero, A. H., Ancilotto, F., & Silvestrelli, P. L. (2006). Lithium adsorption on graphite from density functional theory calculations. *The Journal of Physical Chemistry B*, *110*(30), 14832–14841.

Vlassiouk, I., Smirnov, S., Ivanov, I., Fulvio, P. F., Dai, S., Meyer, H., Lavrik, N. V. (2011). Electrical and thermal conductivity of low temperature CVD graphene: the effect of disorder. *Nanotechnology*, *22*(27), 275716.

Wagner, R. S., & Ellis, W. C. (1964). Vapor liquid solid mechanism of single crystal growth. *Applied Physics Letters*, *4*(5), 89–90.

Wallace, P. R. (1947). The band theory of graphite. *Physical Review*, *71*(9), 622.

Wang, Z. (2009). *First-principles electronic structure theory, Graphene calculations*. Universiteit Van Amterdam.