

# Physical Properties of Novel Two-dimensional Materials and Their Modifications From first-principles studies



### Yierpan Aierken

Supervisor: Prof. François M. Peeters

Advisor: Dr. Ortwin Leenaerts

Dr. Deniz Çakır

Department of Physics, University of Antwerp

This dissertation is submitted for the degree of Doctor of Philosophy

I would like to dedicate this thesis

to my loving parents Arkin and Perwin,

to my beloved wife Adila Dilshat,

to my cherished sons Efran and Wildan.

#### **Declaration**

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. This dissertation contains fewer than 65,000 words including appendices, bibliography, footnotes, tables and equations and has fewer than 150 figures.

Yierpan Aierken April 2017

### Acknowledgements

And I would like to acknowledge ...

### **Abstract**

This is where you write your abstract  $\dots$ 

### **Table of contents**

Li	st of	figures	<b>;</b>	XV
Li	st of	tables		xvii
1	Intro	oductio	on	1
	1.1	Graph	ene	1
		1.1.1	History and prediction	
		1.1.2	Physical properties	1
	1.2	Post-g	graphene Materials	1
		1.2.1	Functionized Graphene	1
		1.2.2	Boron Nitride	1
		1.2.3	Silicene and Germanene	1
		1.2.4	Transition Metal Dichalcogenides	1
	1.3	0D an	d 1D from 2D: buckyballs, nanotubes and nanoribbons	1
	1.4	Synthe	esis methods	1
2	Con	nputati	onal methods	3
	2.1	Theor	y	3
		2.1.1	Density Functional Theory	3
		2.1.2	Exchange-correlation functional	3
		2.1.3	Jocob's ladder	3
	2.2	Impler	mentation	3
		2.2.1	Basis set, Plane wave energy cut-off, K-points	3
		2.2.2	Software Packages	3
3	Gen	eral ph	nysical properties 2D materials	5
	3.1	Struct	ural properties	6
		3.1.1	Layer structure	6
		212	en hybirdization	6

**xii** Table of contents

		3.1.3	Isotropic v.s. Anisotropic monolayer	6
		3.1.4	Multiphase allotropes	6
	3.2	Electro	onic properties	6
		3.2.1	Polar bond	6
		3.2.2	Importance of crystal symmetry	6
		3.2.3	Importance of interlayer interaction	6
		3.2.4	Accurate description from DFT	6
	3.3	Vibrat	ional properties	6
		3.3.1	Phonon dispersion of 2D materials	6
		3.3.2	Dynamic stability from phonon dispersion	6
	3.4	Mecha	anical properties	6
		3.4.1	Elastic and engineering constants	6
		3.4.2	Mechanical stability: Born stability criteria	6
4	Res	ults of	Physical Properties Calculations in Novel 2D materials	7
	4.1	Therm	nal properties	8
		4.1.1	Thermal expansion and anharmonic oscillations	8
		4.1.2	Quasi-harmonic approximation	8
		4.1.3	Helmholtz free energy and specific heat	8
	4.2	Piezo	electric properties	8
		4.2.1	Piezoelectric constants	8
		4.2.2	Importance of internal relaxation	8
	4.3	Carrie	r transport properties	8
		4.3.1	Carrier mobility	8
		4.3.2	Deformation potential theory: non-polar materials	8
		4.3.3	Deformation potential theory: polar materials	8
	4.4	Magne	etic properties	8
		4.4.1	Magnetic ordering	8
	4.5	Batter	y related properties	8
		4.5.1	Principle of Lithium battery	8
		4.5.2	Key quantities and their modelling	8
5	Res	ults of	Physical Properties Modification in Novel 2D materials	9
	5.1	Numb	er of layers and types of stackings	0
		5.1.1	Electronic properties	0
		5.1.2	Vibrational properties	0
	52	Mecha	anical strain 1	n

Table o	of conter	nts	Xiii
	5.2.1	Carrier mobility	10
	5.2.2	Magnetic properties	10
5.3	Adato	m adsorption	10
	5.3.1	Electronic properties	10
5.4	Heter	ostructures	10
	5.4.1	Electronic properties	10
	5.4.2	Li difusion	10
5.5	Defec	t induction	10
	5.5.1	Structural properties	10
	5.5.2	Electronic properties	10
	5.5.3	Magnetic properties	10
6 Co	nclusio	ns	11
Appen	dix A	Appendix	13

### **List of figures**

### **List of tables**

### Introduction

1	.1	Gra	phene
---	----	-----	-------

- 1.1.1 History and prediction
- 1.1.2 Physical properties
- 1.2 Post-graphene Materials
- 1.2.1 Functionized Graphene

Graphane

Fluorographene

- 1.2.2 Boron Nitride
- 1.2.3 Silicene and Germanene
- 1.2.4 Transition Metal Dichalcogenides
- 1.3 0D and 1D from 2D: buckyballs, nanotubes and nanoribbons
- 1.4 Synthesis methods

### **Computational methods**

- 2.1 Theory
- 2.1.1 Density Functional Theory
- 2.1.2 Exchange-correlation functional
- 2.1.3 Jocob's ladder
- 2.2 Implementation
- 2.2.1 Basis set, Plane wave energy cut-off, K-points
- 2.2.2 Software Packages

### General physical properties 2D materials

3. 1 Siructural propertie	3.1	Structural	properties
---------------------------	-----	------------	------------

- 3.1.1 Layer structure
- 3.1.2 sp hybirdization

Coulson's theorem

- 3.1.3 Isotropic v.s. Anisotropic monolayer
- 3.1.4 Multiphase allotropes
- 3.2 Electronic properties
- 3.2.1 Polar bond
- 3.2.2 Importance of crystal symmetry

Clar's theory

- 3.2.3 Importance of interlayer interaction
- 3.2.4 Accurate description from DFT
- 3.3 Vibrational properties
- 3.3.1 Phonon dispersion of 2D materials
- 3.3.2 Dynamic stability from phonon dispersion
- 2.4 Machanical proportion

### Results of Physical Properties Calculations in Novel 2D materials

Til Tiletillai properties	4.1	<b>Thermal</b>	properties
---------------------------	-----	----------------	------------

- 4.1.1 Thermal expansion and anharmonic oscillations
- 4.1.2 Quasi-harmonic approximation
- 4.1.3 Helmholtz free energy and specific heat

### 4.2 Piezoelectric properties

- 4.2.1 Piezoelectric constants
- 4.2.2 Importance of internal relaxation

### 4.3 Carrier transport properties

- 4.3.1 Carrier mobility
- 4.3.2 Deformation potential theory: non-polar materials
- 4.3.3 Deformation potential theory: polar materials

#### 4.4 Magnetic properties

#### 4.4.1 Magnetic ordering

Stoner criterion of ferromagnetism

### 4.5 Battery related properties

### Results of Physical Properties Modification in Novel 2D materials

- 5.1 Number of layers and types of stackings
- 5.1.1 Electronic properties
- 5.1.2 Vibrational properties
- 5.2 Mechanical strain
- 5.2.1 Carrier mobility
- 5.2.2 Magnetic properties
- 5.3 Adatom adsorption
- 5.3.1 Electronic properties
- 5.4 Heterostructures
- 5.4.1 Electronic properties
- 5.4.2 Li difusion
- 5.5 Defect induction
- 5.5.1 Structural properties
- 5.5.2 Electronic properties
- 5.5.3 Magnetic properties

## **Chapter 6 Conclusions**

## Appendix A Appendix