



Ain Shams University
Faculty of Education
Physics Department

*Theoretical Study of Hydrogen Storage capacity in
Different Types of Nano-cones*

Thesis Presented by
Mohammad Ahmed Farea Mohsen Al khateeb

For the Doctor of Philosophy Degree of Teacher Preparation in Science
(Theoretical Physics)

Supervised by

Prof. Dr. Mohammed Ahmed Kamel
Professor of Theoretical Physics
Faculty of Education - Ain Shams University

Dr. Hayam Osman Taha
Associate Professor of Theoretical Physics
Faculty of Education - Ain Shams University

Dr. Rasha Ali Ali Mohammed
Lecturer of Theoretical Physics
Faculty of Education - Ain Shams University

2015

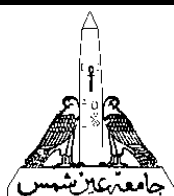
بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

{ قَالُوا سُبْحَانَكَ لَا عِلْمَ لَنَا إِلَّا

مَا عَلَّمْتَنَا إِنَّكَ أَنْتَ الْعَلِيمُ

{ الْحَكِيمُ

صَدَقَ اللَّهُ الْعَظِيمُ



Ain Shams University
Faculty of Education
Physics Department

Researcher Name: *Mohammed Ahmed Farea Mohsen*
Al-Khateeb

Title of the thesis: *Theoretical Study of Hydrogen Storage*
capacity in Different Types of Nano-cones.

Submitted to: *Physics Department, Faculty of Education,*
Ain Shams University

Supervisors:

1- Prof. Dr. Mohammed Ahmed Kamel

2- Dr. Hayam Osman Taha

3- Dr. Rasha Ali Ali Mohammed

Approval Sheet

Title : " *Theoretical Study of Hydrogen Storage capacity in Different Types of Nano-cones* "

Candidate: Mohammed Ahmed Farea Mohsen Al-Khateeb

Degree : Doctor of Philosophy degree of Teacher Preparation
in Science

(Physics)

Board of Advisors

Approved by

1. Prof. Dr/ Mohammed Ahmed Kamel

Prof. of Theoretical Physics
Faculty of Education, Ain Shams University

2. Dr/ Hayam Osman Taha

Associate Professor of Theoretical Physics
Faculty of Education, Ain Shams University

3. Dr/ Rasha Ali Ali Mohammed

Lecturer of Theoretical Physics
Faculty of Education, Ain Shams University

Date of presentation: / / 2015

Post graduate studies:

Stamp: / /

Date of approval: / / 2015

Approval of Faculty Council: / / 2015

Approval of University Council: / / 2015

Contents

	Page
Acknowledgement	i
Special Acknowledgement	iii
List of Tables	iv
List of Figures	vi
Abbreviations	Xvi
Abstract	xvii
Summary	xviii

Chapter I **Introduction**

1.1 Current Situation of Energy Sources.....	1
1.2 Hydrogen as Clean, Efficient, Renewable Energy Carrier	2
1.3 Scientific Challenges And Fundamental Research Need: of on-board Hydrogen Storage.....	4
1.4 Generating Green Electricity.....	7
1.5 carbon.....	11
1.6 Nanocons	12
1.7 Defects.....	16
1.7.1 Point Defects.....	17
1.7.2 Line Defects.....	18

Chapter II **Theoretical background**

2.1 The Electronic Problem.....	19
2.1.1 Born-Oppenheimer Approximation.....	20
2.1.2 Antisymmetric or Pauli Exclusion Principle.....	21
2.2 Orbital and Slater Determinants.....	22
2.2.1 Spin Orbitals and Spatial Orbitals.....	22
2.2.2 Hartree Product.....	23
2.2.3 Slater Determinants.....	25
2.3 Hartree-Fock Theory.....	26

2.3.1 Hartree-Fock Equations.....	26
2.3.2 Fock operator.....	29
2.4 Density Functional Theory.....	30
2.4.1 Local Density Approximation.....	32
2.5 Ab Initio Modelling Program Packages.....	33
2.5.1 Gaussian 03 Package.....	33
2.5.2 Basis Sets.....	34

Chapter III

Literature review

Literature review.....	38
------------------------	----

Chapter IV

Pure Carbon Nanocones (CNCs)

4.1 Introduction	50
4.2 Computational Methods	50
4.3 Results.....	51
4.3.1 Geometric structures	51
4.3.2. Surface reactivity	57
4.3.3 Energy gaps	59
4.3.4 HOMOs and LUMOs.....	61
4.3.5 Density of States.....	68
4.4 Conclusion	73

Chapter V

Pure Boron Nitride Nanocones (BNNCs)

5.1 Introduction.....	75
-----------------------	----

Contents

5.2 Computational Methods	75
5.3 Results	76
5.3.1 Geometric structures	76
5.3.2 Surface reactivity	84
5.3.3 Energy gaps	87
5.3.4 HOMOs and LUMOs	89
5.3.5 Density of States	99
5.4 Conclusion.....	107

Chapter VI

Hydrogenated Carbon Nanocones (CNCs)

6.1 Introduction	109
6.2 Computational Methods	110
6.3 Results	111
6.3.1 Geometric structures.....	111
6.3.2 Adsorption energy of mono-hydrogenation CNCs...	117
6.3.3 Surface reactivity	119
6.3.4 Energy gaps	121
6.3.5 HOMOs and LUMOs	123
6.3.6 Density of States	131
6.4 Conclusions	138

Chapter VII
Hydrogenated Boron Nitride Nanocones
(BNNCs)

7.1 Introduction.....	139
7.2 Computational Methods.....	140
7.3 Results.....	140
7.3.1 Geometric structures.....	140
7.3.2 Adsorption energy of mono-hydrogenation BNNCs...	157
7.3.3 The surface reactivity of mono-hydrogenation BNNCs	161
7.3.4 Energy gaps of mono-hydrogenation BNNCs	165
7.3.5 HOMOs and LUMOs of mono-hydrogenation BNNCs...	169
7.3.6 Density of states for mono-hydrogenation BNNCs.....	179
7.4 Conclusions.....	182
 Conclusions.....	 183
 References.....	 187
Arabic Summary	

Acknowledgment

***Before all and above all, many thanks to Allah,
the lord of all beings.***

I am greatly privileged and honored to have Prof. Dr/ ***Mohammed Ahmed Kamel, Dr/ Hayam Osman Taha*** and Dr/ ***Rasha Ali Ali Mohammed*** as my supervisors.

My deepest thanks and gratitude to Prof. Dr/ ***Mohammed Ahmed Kamel***, Professor of Theoretical Physics, Faculty of Education, Ain Shams University, for his everlasting encouragement, continuous supervision, valuable criticism and fruitful advice which can never be forgotten.

My deepest thanks and gratitude to, ***Dr/ Hayam Osman Taha*** Associate professor of Theoretical Physics, Faculty of Education, Ain Shams University, for her continuous supervision, valuable suggestions and everlasting encouragement during this work.

My deepest thanks and gratitude to, ***Dr/ Rasha Ali Ali Mohammad*** Lecturer of Theoretical Physics, Faculty of Education, Ain Shams University, for her continuous supervision, valuable suggestions and everlasting encouragement during this work.

Acknowledgment

Sincere thanks and appreciation to Prof. Dr/ **Mahmoud Yassin**, head of Physics Department, Faculty of Education, Ain Shams University for her everlasting encouragement.

Finally, I would like to thank my parents, my wife (Nagla'a) and my boys Ezz Adeen, Madian, Rawi and Raba'a for their continuous assistance in my life.

Special Acknowledgement

My deepest thanks and gratitude to. Dr/ ***Ahlam Abd El-Monem Ahmed El-Barbary***, Associate Professor of Theoretical Physics, Faculty of Education, Ain Shams University, for her suggestion of the problem of research point before departure to Saudi Arabia, (Physics Department, Faculty of Science, Jazan University, KSA), Also for her continuous discussions through calculations, writing my papers and finishing up my thesis. Many thanks for her exerted effort and fruitful help, throughout this research that will never forget and I wish if her name it would be included with the supervisions and wishing her successful academic life.

List of Tables

	Page
Table (4.1): The calculated surface reactivities for CNCs with disclination angles 60^0 , 120^0 , 180^0 , 240^0 and 300^0 . All dipole moments given by Debye.	58
Table (4.2): The calculated energy gaps (E.g) for CNCs with disclination angles 60^0 , 120^0 , 180^0 , 240^0 and 300^0 . All energy gaps given by ev.	60
Table (5.1): The calculated surface reactivities for BNNCs with disclination angles 60^0 , 120^0 , 180^0 , 240^0 and 300^0 . All dipole moments given by Debye.	86
Table (5.2): The calculated energy gaps (E.g) for BNNCs with disclination angles 60^0 , 120^0 , 180^0 , 240^0 and 300^0 . All energy gaps given by ev.	88
Table (6.1): The calculated adsorption energy of mono-hydrogenation CNCs with disclination angles 60^0 , 120^0 , 180^0 , 240^0 and 300^0 at three different sites H^{S1} , H^{S2} and H^{S3} . All energies are given by ev.	118
Table (6.2): The configuration structures and dipole moments of mono- hydrogenated CNCs with disclination angles 60^0 , 120^0 , 180^0 , 240^0 and 300^0 at three different sites H^{S1} , H^{S2} and H^{S3} . All dipole moments are given by Debye.	120
Table (6.3): The configuration structures and dipole moments of mono- hydrogenated CNCs with disclination angles 60^0 , 120^0 , 180^0 , 240^0 and 300^0 at three different sites H^{S1} , H^{S2} and H^{S3} . All energies are given by ev.	122
Table (7.1): The configuration structures and the adsorption energy of mono- hydrogenated BNNCs-type1 and type2 for disclination angles 120^0 and 240^0 . All energies are given by eV.	159
Table (7.2): The configuration structures and the adsorption energy of mono- hydrogenated BNNCs-M1 type1 and BNNCs-M1 type2 for disclination angles 60^0 , 180^0 and 300^0 . All energies are given by eV.	160

List of Tables

Table (7.3): The configuration structures and the adsorption energy of mono- hydrogenated BNNCs-M2 type1 and BNNCs-M2 type2 for disclination angles 60° , 180° and 300° . All energies are given by eV.	161
Table (7.4): The configuration structures and the dipole moments of mono-hydrogenated BNNCs-Type1 and BNNCs-Type2 for disclination angles 120° and 240° . The dipole moment is given by Debye.	162
Table (7.5): The configuration structures and the dipole moments of mono-hydrogenated BNNCs-M1-Type1 and BNNCs-M1-Type2, for disclination angles 60° , 180° and 300° . The dipole moment is given by Debye.	163
Table (7.6): The configuration structures and the dipole moments of mono-hydrogenated BNNCs-M2-Type1 and BNNCs-M2-Type2, for disclination angles 60° , 180° and 300° . The dipole moment is given by Debye.	164
Table (7.7): The configuration structures and the energy gaps of mono-hydrogenated BNNCs-Type1 and BNNCs-Type2 for disclination angles 120° and 240° . Energies are given by eV.	166
Table (7.8): The configuration structures and energy gaps of mono-hydrogenated BNNCs-M1-Type1 and BNNCs-M1-Type2, for disclination angles 60° , 180° and 300° . Energies are given by eV.	167
Table (7.9): The configuration structures and energy gaps of mono-hydrogenated BNNCs-M2-Type1 and BNNCs-M2-Type2, for disclination angles 60° , 180° and 300° . Energies are given by eV.	168

<u><i>List of Figures</i></u>	Page
Figure(1.1): (a) a fuel cell generates electricity by reacting oxygen, hydrogen ions and electrons. (b) the hydrogen ions generated at the anode are swept through a membrane to the cathode. This membrane is impermeable to electrons generated at the anode.	9
Figure 1.2 : Nanocones are carbon-based structures formed by introducing 600 positive disclination defects in two-dimensional graphene sheets.	14
Figure 1.3: Schematic representations of molecular models of carbon nanocones (a) cone60, (b) cone120, (c) cone180, (d) cone240, (e) and (f) cone300.	16
Figure 1.4 Point Defects.	17
Figure 1.5 Line defects (Dislocations)	18
Figure 4.1: Structures of carbon nanocones with disclination angle 60^0 for (a) $C_{45}H_{15}$, (b) $C_{80}H_{20}$, (c) $C_{115}H_{25}$ and (d) $C_{170}H_{30}$.	52
Figure 4.2: Structures of carbon nanocones with 120^0 angle for (a) $C_{36}H_{12}$, (b) $C_{56}H_{16}$, (c) $C_{92}H_{20}$ and (d) $C_{136}H_{24}$.	53
Figure 4.3: Structures of carbon nanocones with 180^0 angle for (a) $C_{48}H_{12}$, (b) $C_{75}H_{15}$, (c) $C_{102}H_{18}$ and (d) $C_{141}H_{21}$.	54
Figure 4.4: Structures of carbon nanocones with 240^0 angle for (a) $C_{28}H_8$, (b) $C_{46}H_{10}$, (c) $C_{68}H_{12}$ and (d) $C_{94}H_{14}$.	55
Figure 4.5: Structures of carbon nanocones with 300^0 angle for (a) $C_{23}H_5$, (b) $C_{34}H_6$, (c) $C_{58}H_8$ and (d) $C_{90}H_{10}$.	56
Figure 4.6: The obtained HOMOs and LUMOs of carbon nanocones with disclination angle 60^0 for (a) $C_{45}H_{15}$, (b) $C_{80}H_{20}$, (c) $C_{115}H_{25}$ and (d) $C_{170}H_{30}$	62
Figure 4.7: The obtained HOMOs and LUMOs of carbon nanocones with disclination angle 120^0 for (a) $C_{36}H_{12}$, (b) $C_{56}H_{16}$, (c) $C_{92}H_{20}$ and (d) $C_{136}H_{24}$.	63

Figure 4.8: The obtained HOMOs and LUMOs of carbon nanocones with disclination angle 180^0 for (a) $C_{48}H_{12}$, (b) $C_{75}H_{15}$, (c) $C_{102}H_{18}$ and (d) $C_{141}H_{21}$.	65
Figure 4.9: The obtained HOMOs and LUMOs of carbon nanocones with disclination angle 240^0 for (a) $C_{28}H_8$, (b) $C_{46}H_{10}$, (c) $C_{68}H_{12}$ and (d) $C_{94}H_{14}$.	66
Figure 4.10: The obtained HOMOs and LUMOs of carbon nanocones with disclination angle 300^0 for (a) $C_{23}H_5$, (b) $C_{34}H_6$, (c) $C_{58}H_8$ and (d) $C_{90}H_{10}$.	67
Figure 4.11: The calculated total density of states for CNCs with disclination angle 120^0 for (a) $C_{36}H_{12}$, (b) $C_{56}H_{16}$, (c) $C_{92}H_{20}$ and (d) $C_{136}H_{24}$.	68
Figure 4.12: The calculated total density of states for CNCs with disclination angle 120^0 for (a) $C_{36}H_{12}$, (b) $C_{56}H_{16}$, (c) $C_{92}H_{20}$ and (d) $C_{136}H_{24}$.	69
Figure 4.13: The calculated total density of states for CNCs with disclination angle 180^0 for (a) $C_{48}H_{12}$, (b) $C_{75}H_{15}$, (c) $C_{102}H_{18}$ and (d) $C_{141}H_{21}$.	70
Figure 4.14: The calculated total density of states for CNCs with disclination angle 240^0 for (a) $C_{28}H_8$, (b) $C_{46}H_{10}$, (c) $C_{68}H_{12}$ and (d) $C_{94}H_{14}$.	71
Figure 4.15: The calculated total density of states for CNCs with disclination angle 300^0 for (a) $C_{23}H_5$, (b) $C_{34}H_6$, (c) $C_{58}H_8$ and (d) $C_{90}H_{10}$.	72
Figure (5.1): Structures of boron nitride nanocones with 60^0 angle for M1 (a) $B_{21}N_{24}H_{15}$, (b) $B_{38}N_{42}H_{20}$, (c) $B_{56}N_{42}H_{25}$ and (d) $B_{83}N_{87}H_{30}$.	77
Figure (5.2): Structures of Boron Nitride Nanocones with 60^0 angle for M2 (a) $B_{24}N_{21}H_{15}$, (b) $B_{42}N_{38}H_{20}$, (c) $B_{42}N_{56}H_{25}$ and (d) $B_{87}N_{83}H_{30}$.	78
Figure(5.3): : Structures of boron nitride nanocones with 120^0 angle for structures (a) $B_{18}N_{18}H_{12}$, (b) $B_{28}N_{28}H_{16}$, (c) $B_{46}N_{46}H_{20}$ and (d) $B_{68}N_{68}H_{24}$.	79