

*Ain Shams University
Faculty of Education
Physics Department*

Theoretical Investigation of Hydrogen Storage Capacity in Defected Carbon Materials

THESIS

*Submitted in partial fulfillment
of the requirement for the Master degree of
Teacher Preparation in Science (Physics)*

By

Mohamed Ahmed Farea Mohsen Al Khateeb

To

***Physics Department
Faculty of Education
Ain Shams University***

2011

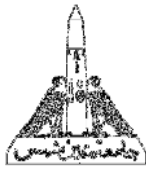
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Title of the thesis: *Theoretical Investigation of Hydrogen*
Storage Capacity in Defected Carbon Materials

Submitted to: *Physics Department, Faculty of Education,*
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Date of presentation: / / 2011

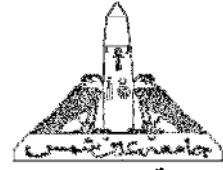
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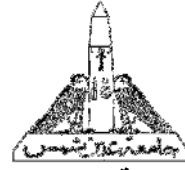
دراسة نظرية لسعة تخزين الهيدروجين في المواد الكربونية المشوهة

رسالة
مقدمة للحصول على ماجستير إعداد المعلم
في العلوم (فيزياء)

مقدمة من
محمد أحمد فارح محسن الخطيب

إلى
قسم الفيزياء
كلية التربية
جامعة عين شمس

٢٠١١



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كلية التربية
قسم الفيزياء

رسالة ماجستير

اسم الطالب : محمد أحمد فارح محسن الخطيب

عنوان الرسالة : دراسة نظرية لسعة تخزين الهيدروجين في المواد الكربونية المشوهة

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تاريخ البحث: / / ٢٠١١

الدراسات العليا

أجيزت الرسالة بتاريخ

/ / ٢٠١١

موافقة مجلس الجامعة

/ / ٢٠١١

ختم الإجازة

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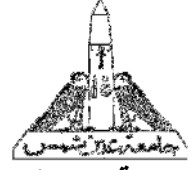
/ / ٢٠١١



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صفحة العنوان

اسم الطالب : محمد أحمد فارح محسن الخطيب
الدرجة العلمية : الماجستير في اعداد المعلم في الفيزياء
القسم التابع له : الفيزياء
اسم الكلية : التربية
الجامعة : عين شمس
سنة التخرج : ٢٠٠١
سنة المنح : ٢٠١١



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الإهداء

أهدي هذا العمل إلى:

وطنــــي الذي ليس كمثلـه وطن.....وفاءً بالجميل،

روح أمي الطاهرة.....دعاءً ورحمة،

روح والدي الطاهرة.....دعاءً ورحمة،

زوجتي الغالية، واولاديحبا، وتقديراً،

كل من اسدل لي معروفاً وانا ر لي الطريق.....عرفاناً بالجميل،

الباحثون في محراب العلم.....دعاءً، وتوفيقاً.

Abstract

This work is classified as follows:

Hydrogen is abundant, uniformly distributed throughout the Earth's surface and its oxidation product (water) is environmentally benign. Owing to these features, it is considered as an ideal synthetic fuel for new energetic matrix (renewable, secure and environmentally friendly) that could allow a sustainable future development. However, for this prospect to become a reality, efficient ways to produce, transport and store hydrogen still need to be developed. In this thesis, theoretical studies of a number of potential hydrogen storage materials have been performed using Hartree Fock (HF) and Density Functional (DFT) theories with applying 3-21G and 6-31G basis sets. The hydrogen storage in two different types of carbon materials, pristine- graphite and carbon (5,5) nanotubes, will be investigated. Then, we will explore the role of defects and doping on the cavity of hydrogen storage. Therefore, we will study isolated, mono- and di- vacancy defected graphite and (5,5) carbon nanotubes. The effect of boron and nitrogen doping in graphite and (5,5) carbon nanotubes will be also studied. Mulliken analysis, electron distribution and molecular orbitals will be applied to analyze the obtained results.

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