Theoretical study on the defects and their dynamics in multi-wall carbon nanotube

2007 Fiscal Year Final Research Report Summary

Theoretical study on the defects and their dynamics in multi-wall carbon nanotube

Research Project

Project/Area Number

17510097

Research Category

Grant-in-Aid for Scientific Research (C)

Allocation Type

Single-year Grants

Section

一般

Research Field

Nanomaterials/Nanobioscience

Research Institution

Kanazawa University

Principal Investigator

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Project Period (FY)

2005 – 2007

Keywords

nano-technology / electronics / carbon nano-tube / graphene / inherent defect / magic number / density functional theory / iron nano-wire

Research Abstract

energy, compared with the atomic vacancy defect.
We have researched the set of chiralities for the double walled (DW) CNT which corresponds to the experimentally observed one. For the DWCNT (13, 0)@(22, 0), we have obtained the electronic structure. We have also studied the electronic structure of the CNTs which include the Fe atomic wire. At the stable geometry in which the Fe atoms form a straight wire, the Fe wire was found to be located on the wall. We have obtained a ferromagnetic alignment and a novel anti-ferromagnetic one in Fe magnetic configurations as low energy states. The anti-ferromagnet consists of the two ferromagnetic dimers which couple in anti-parallel alignment.

Research Products (84 results)

All | 2008 | 2007 | 2006 | 2005

All | Journal Article (38 results) (of which Peer Reviewed: 25 results) | Presentation (46 results)

[Journal Article] 「電子状態をあらわに考慮した分子動力学シミュレーションの基礎(4):第一原理分子動力学シミュレーションなど」 2008

[Journal Article] Magnetic anisotropy of Fe/Pt(001)and Pt/Fe/Pt(001)using a first-principles approach 2008

[Journal Article] Oxygen at High Pressures: Theoretical Approach to Monoatomic Phases 2007

[Journal Article] Magnetic Anisotropies of Iron on the Pt(111)Surface, 2007

[Journal Article] Development of Fully Relativistic Pseudopotentials and Application to a Thin Magnetic Film on the Metal 2007

[Journal Article] Magnetic Anisotropies of Iron on the Low Index Platinum Surface 2007

[Journal Article] Electronic Structure and Magnetism of Fe-Wire in Carbon Nanotubes 2007

[Journal Article] Structure and Magnetism in Carbon Nanotubes Including Magnetic Wire 2007

[Journal Article] Structure and Electronic Properties of Heterojunction of Single Wall Carbon Nanotube and TiC Cluster 2007

[Journal Article] Formation of a Five-Seven Pair Couple Defect in Double-Walled Carbon Nanotubes under Bending Deformation 2007

[Journal Article] Magic Numbers of Graphene Multivacancies 2007

[Journal Article] 「電子状態をあらわに考慮した分子動力学シミュレーションの基礎(1):第一原理分子動力学シミュレーションなど」 2007

[Journal Article] 「電子状態をあらわに考慮した分子動力学シミュレーションの基礎(2):第一原理分子動力学シミュレーションなど」 2007

[Journal Article] 「電子状態をあらわに考慮した分子動力学シミュレーションの基礎(3):第一原理分子動力学シミュレーションなど」 2007

[Journal Article] Comparative Study on the Atomic and Electronic Structures of P and Bi Nanofilms 2007

[Journal Article] Origin of Flat Morphology and High Crystallinity of Ultrathin Bismuth Films 2007

[Journal Article] STM/STS studies of the initial stage of growth of ultra-thin Bi films on 7×7-Si(111)surface 2007

[Journal Article] Electronic Structure and Magnetism of Fe-Wire in Carbon Nanotubes 2007

[Journal Article] Structure and Magnetism in Carbon Nanotubes Including Magnetic Wire 2007

[Journal Article] Magic Numbers of Graphene Multivacancies 2007

[Journal Article] Stability of the quasicubic in the initial stage of the growth of bismuth films on Si(111)-7×7 2006

[Journal Article] Atomic Geometry and Stability of Mono-, Di-and Trivacancies in Graphene 2006

[Journal Article] Role of spin-orbit coupling and hybridization effects in the electronic structure of ultrathin Bi films 2006

[Journal Article] Origin of n type conductivity in wide gap semiconductors studied by μ SR 2006

[Journal Article] Isolated hydrogen center in wide gap semiconductors studied by μs 2006

[Journal Article] Atomic Geometry and Stability of Mono-, Di- and Tri-vacancies in Graphene 2006

[Journal Article] Role of spin-orbit coupling and hybridization effects in the electronic structure of ultrathin Bi films 2006

[Journal Article] Structure and Magnetic Properties of Iron Chains Encapsulated in Tubal Carbon Nano Capsules 2005

[Journal Article] Structure and Magnetism of Anion Iron Oxide Clusters Fe_nO_m(n=3,4) 2005

[Journal Article] Electronic structure and magnetism at the active site in ferredoxin: ab initio approach to(Fe_2S_2)^<2+>complex with the 1st peptide shell 2005

[Journal Article] Fully Relativistic Two-Component-Spinor Approach in the Ultra-Soft-Pseudopotential Planewave Method 2005

[Journal Article] シリコン表面上の半金属Bi 超薄膜の同素変態 2005

[Journal Article] Strong lateral growth and crystallization via two-dimensional allotropic transformation of semi-metal Bi film 2005

[Journal Article] Self-energy correction to momentum-density distribution of positron-electron pairs 2005

[Journal Article] Structure and Magnetic Properties of Iron Chains Encapsulated in Tubal Carbon Nano Capsules 2005

[Journal Article] Fully Relativistic Two-Component-Spinor Approach in the Ultra-Soft-Pseudopotential Planewave Method 2005

[Journal Article] Self-energy correction to momentum-density distribution of positron-electron pairs 2005

[Journal Article] Strong lateral growth and crystallization via two-dimensional allotropic transformation of semi-metal Bi film 2005

[Presentation] 白金表面上鉄鎖の電子状態と磁気異方性 2008

[Presentation] 鉄白金クラスターの原子構造と磁気異方性 2008

[Presentation] スピン軌道結合で分裂した表面電子バンドと表面緩和による磁気異方性変化 2008

[Presentation] 5-7員環の対によるカーボンナノチューブの曲げ変形 2008

[Presentation] Development of fully relativistic pseudopotentials and application to the sixth-row elements of the periodic table 2008

[Presentation] Electronic structures and magnetic anisotropies of thin iron films on platinum surfaces 2008

[Presentation] First-principles molecular dynamics method with noncollinear magnetism 2008

[Presentation] Quantum Mechanical Simulation of Electronic Structures of Defects in Carbon Materials Computational Science 2008

[Presentation] 5-7員環の対によるカーボンナノチューブの曲げ変形 2008

[Presentation] 鉄原子によるカーボンナノチューブ端の電子状態の変化 2007

[Presentation] 白金(111)面および(664)微斜面上鉄原子鎖の磁気異方性 2007

[Presentation] スピン軌道相互作用を考慮した擬ポテンシャルの開発 2007

[Presentation] 鉄原子が吸着したカーボンナノチューブ端の電子状態と分子動力学シミュレーション 2007

[Presentation] 白金表面上に担持された鉄鎖の電子状態と磁気異方性 2007

[Presentation] 小さな鉄白金磁性クラスターの構造と磁気異方性 2007

[Presentation] Development of fully relativistic pseudopotentials and application to the elements of the sixth row in the periodic table 2007

[Presentation] Atomic structures of graphene adatom and its aggregation 2007

[Presentation] Bistability of Ultarthin Bi Films 2007

[Presentation] Two-component density functional calculation on positron annihilation in avariety of crystals 2007

[Presentation] Water Effect on Infrared Spectra of DNA: First-Principles Study 2007

[Presentation] Development of fully relativistic pseudopotentials and application to the elements of the sixth row in the periodic table 2007

[Presentation] 5-7員環対が生成したカーボンナノチューブの曲げ変形に対する安定性 2007

[Presentation] カーボンナノチューブ中の鉄クラスターの磁気構造、原子構造および電子状態 2007

[Presentation] 「スピン軌道相互作用を考慮した擬ポテンシャルの開発と表面系への応用」 2007

[Presentation] グラフェン固有欠陥の拡散と集合 2007

[Presentation] カーボンナノチューブ端における電子状態と磁気モーメント 2007

[Presentation] 白金表面上鉄薄膜の磁気異方性 2007

[Presentation] Pt(111)および(001)表面上Fe薄膜の構造と磁気異方性 2007

[Presentation] Two-component density functional calculations on lifetimes of positrons in a variety of crystals 2007

[Presentation] Car-Parrinello Molecular Dynamics Method with Noncollinear Magnetism 2007

[Presentation] グラフェン・アドアトムの第一原理計算 2007

[Presentation] グラフェン・アドアトムの第一原理計算 2007

[Presentation] 白金(111)表面上の鉄薄膜における構造と磁気異方性エネルギー 2007

[Presentation] カーボンナノチューブ端の電子状態と分子動力学シミュレーション 2007

[Presentation] Structure and Magnetism in Carbon Nanotubes Including Magnetic Wire 2006

[Presentation] 「固体表面と生体分子の第一原理計算」, 2006

[Presentation] グラフェン固有欠陥の構造・安定性・拡散 2006

[Presentation] 高圧固体酸素の構造に関する理論的研究 2006

[Presentation] Magnetic anisotropies of cobalt and iron on the platinum(111)surface 2006

[Presentation] 擬ポテンシャル法による表面磁気異方性エネルギーの見積もり **2006**

[Presentation] グラフェン多原子空孔における5員環の生成 **2006**

[Presentation] グラフェン固有欠陥の第一原理計算 **2006**

[Presentation] Structure and Noncollinear Magnetism in Liquid Oxygen : First-Principles Molecular Dynamics Study **2006**

[Presentation] 第19回分子シミュレーション討論会 **2005**

[Presentation] Atomic structures and electronic properties of Bi nanofilms **2005**

[Presentation] 曲げ変形によるカーボンナノチューブの構造欠陥の生成の計算 **2005**

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