ELECTRONIC PROPERTIES OF CARBON NANOTUBES FOR GAS SENSING APPLICATION THROUGH DFT APPROACH

Report submitted to SASTRA Deemed to be University

As per the requirement for the course

RESEARCH CREDIT

Submitted by

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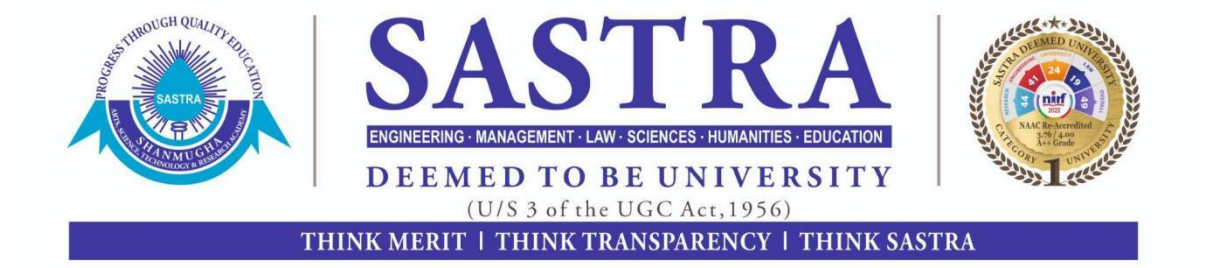
May 2024



SCHOOL OF ELECTRICAL AND ELECTRONICS ENGINEERING

THANJAVUR, TAMIL NADU, INDIA – 613 401

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Signature of Project Supervisor :

Name with Affiliation :

Date :

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Examiner 1 **Examiner 2**

ACKNOWLEDGEMENTS

We would like to thank our Honorable Chancellor **Prof. R. Sethuraman** for providing us with an opportunity and the necessary infrastructure for carrying out this project as a part of our curriculum. We would like to thank our Honorable Vice-Chancellor **Dr. S. Vaidhyasubramaniam** and **Dr. S. Swaminathan**, Dean, Planning & Development, for their encouragement and strategic support at every step of our college life.

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We would like to extend our gratitude to all the teaching and non-teaching faculties of the School of Electrical and Electronics who have either directly or indirectly helped us in the completion of the project.

We gratefully acknowledge all the contributions and encouragement from my family and friends resulting in the successful completion of this project. We thank you all for providing me with an opportunity to showcase my skills through this project.

ABSTRACT

Simulating Carbon Nanotube to study the electrical properties with the help of Quantumwise Atomistix Toolkit (ATK) reveals significant alterations in density of states, electric current, and total energy in the presence of target molecules. The findings suggest converting these simulations into physical sensor for cost-effective and for the need of compact integration sensing solution. In the quest for affordable and reliable gas sensors, graphene stands out for its exceptional properties, making it ideal for modern applications. Based on its properties such as the conductivity, light transmittance and thermal conductivity.

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Abbreviations

LDA	Local Density Approximation
GGA	Generalized Gradient Approximation
CNT	Carbon Nanotube
DFT	Density Functional Theory
PGNFs	Pristine Graphene Nanotubes
SWCNT	Single Walled Carbon Nanotube
DoS	Density of States

CHAPTER 1
INTRODUCTION

The study of environmental-based gases has been on an exponential rise, specific to its sensitivity. When it comes to detecting dangerous chemicals in the gaseous state by nature, it could be done so with the help of these gas-sensitive sensors, thereby having constant support to provide an alert.

Due to the specific optical and electrical properties, Carbon-based materials have started to play an important role in behaving as a Gas Sensor. With the use of QuantumATK, the rapid device simulation algorithm helps in giving maximum accuracy concerning the material properties and DFT Calculations.

Starting from designing the molecule with the Builder to sending it to the Script Generator to use the Analysis tools for receiving the Density of States and therefore having the results be generated either as textual representation and also a 2D Plot with the density of states for each respective orbitals of electrons versus the energy level of electron in eV, the functionalities can be done with QuantumATK.

1.2 MOTIVATION

The motivation for research on making Carbon Nanotubes to work as a Gas Sensor is due to its reverse change in nature of the Density of States when exposed to the vapour of chemicals in a gaseous state. This was achieved when determining the simulation of Carbon Nanotubes using QuantumATK and finding the analysis of the Density of States.

Most importantly, while conducting a study on a Single-walled Carbon Nanotube (SWCNT), there exists an interaction between the target molecule to be detected and the atoms of the Carbon Nanotube where a unique transfer of charges took place during the interaction between the molecules.

It can also be attributed to how the lifetime of the charge carriers present in CNT also had a change. Thereby, when even a small amount of target molecule is being exposed, due to the high sensitivity and absorption property of the Carbon Nanotube, the reverse nature of the Density of States was observed.

1.3 SUMMARY OF THE BASE PAPER

Title: DFT study of adsorption properties of the ammonia on both pristine and Si-doped graphene Nano flakes

Author: Kareem H. Bardan, Fouad N. Ajeel, Mohammed H. Mohammed, Alaa M. Khudhair, Ali Ben Ahmed
Publisher: IEEE
Year: 2023
DOI: 10.1016

This paper discusses the research on designing a novel material type to help build an application of a Nano-based sensor where the existing bonding and interaction from both the molecules – target molecule and carbon nanotube is being carried out. The study of calculation is based upon the chemical properties with the use of the density functional theory (DFT) method thereby the execution of absorption of NH3 ammonia molecules over the Pristine Graphene Nano flakes. (PGNFs) and Silicon-doped Graphene Nano flakes (Si-GNFs).

Two distinct inferences were made with the ammonia molecule being physically absorbed on the pristine graphene Nano flakes whereas, on the other hand, the Chemisorption of ammonia molecule takes place on the silicon-doped graphene Nano flakes. Even when the time taken by ammonia to be absorbed is very little, pure PGNFs are made to interact with NH3, and the recovery time to distinguish both is high due to the highly sensitive nature of PGNFs and NH3.

But the Silicon doped GNFs having more absorption level of significance with regards to ammonia, added to an increased conductivity in terms of electrical, Si-GNF Cluster is an

excellent probable for having it used as a Nano-based sensor due to the prominent chemisorption process of Ammonia towards the Silicon doped graphene Nano flakes. Hence, the research paper further concludes by choosing silicon-doped graphene Nano flakes to be a better primary molecule than PGNFs when we try detecting Ammonia.

1.4 RESEARCH GAP

While arriving at proving the validity of the property, simulations and analysis of the Carbon Nanotube were required. From the concept of device physics, the Density of States (DoS), is an important characteristic which tells us about the change in state density to assess the target molecule to be detected.

Even though the properties are varied when CNT is exposed to the gas vapours, some instances such as molecules like Water (H2O) and Carbon Monoxide (CO) don't show the desired change in their characteristics when subjected to exposure. This led to a Research Gap where once again carbon nanotube was termed for not being able to be used as a sensitive Gas detector since such molecules cannot be absorbed to the surface of the carbon nanotube. Since, when an intrinsic carbon nanotube interacts with carbon monoxide or water molecules, an unbalanced low net transfer of electrons takes place.

Hence, doping with N2 is an option to make the net electron transfer maximum and to establish a strong bonding. Also, an insight into the stability and other electron properties such as Density of States the method of behaviour of a solid when subjected to varying environmental surroundings.

1.5 PROBLEM STATEMENT

Study of Carbon Nanotube Gas Sensor by DFT (density functional theory) Approach. Developing a Nano sensor-based application with the relevant study on its properties.

1.6 OBJECTIVE

The overall objective of the work revolves around the intake of a great depth of understanding of the electronic properties of Carbon Nanotubes through the DFT Approach using QuantumATK.

The objective is made as a two-stage with the first analyzing the electron property of the carbon nanotube before and after absorption, that is, introducing the target molecule. Simulating carbon nanotube sensors with the help of Quantumwise Atomistix Toolkit (ATK) that reveal significant alterations under the density of states, in the presence of target molecules.

From the findings taken from the study, consideration of converting received simulations to establish it as a cost-effective physical sensor could also be made the solution for compact sensing solution. In searching for an affordable and reliable gas sensor, Graphene stood out for its ideal properties to use for modern applications.

QuantumATK comes in hand off to a much tool to handle the designing of the nanotube structure, adjusting the parameters involved such as the approximation technique chosen to be GGA – Generalized Gradient Approximation which modifies by correction of over calculated binding energy of LDA which is an essential process required to publish the analysis for density of states before and after the absorption of Gas molecules.

1.7. CARBON NANOTUBE

1.7.1 PROPERTIES

CNT	Carbon Nanotube
Density	1.3 to 1.4 g/cm^3
Appearance	Black
Molecular Weight	12.01g
Odour	Rotting
Solubility	Insoluble

Table-1: Properties of Carbon Nanotube

1.7.2. STRUCTURE

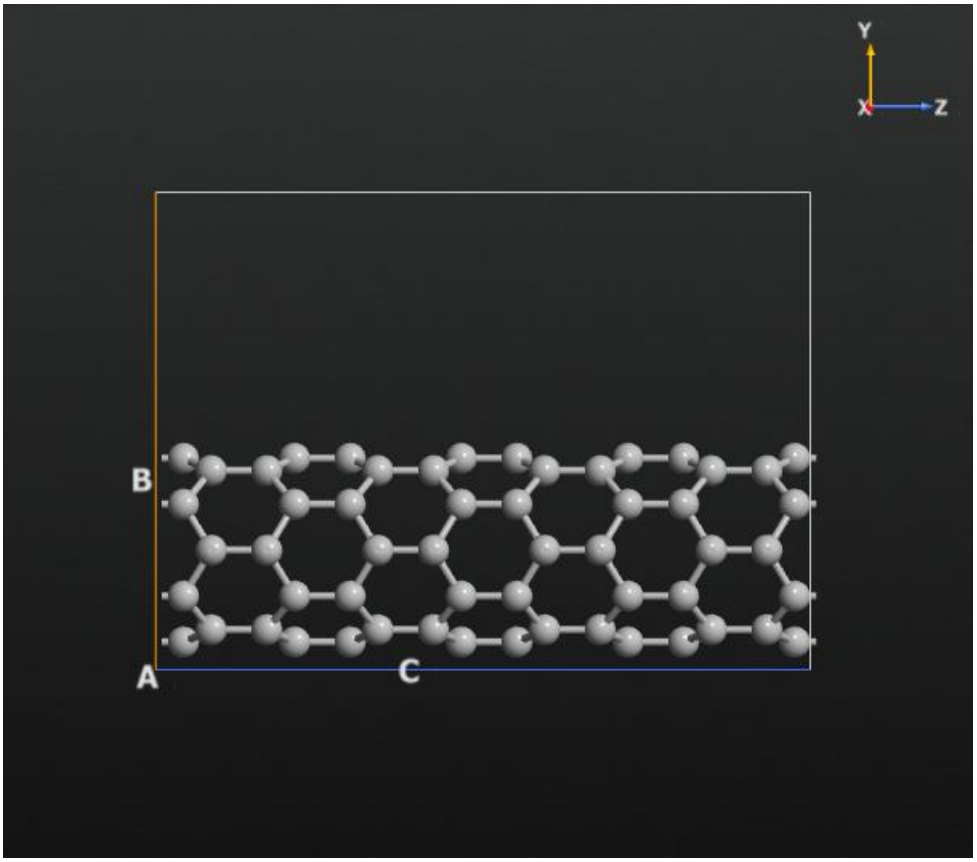

Fig .1 Structure of Carbon Nanotube built using QuantumATK.

CHAPTER II
LITERATURE SURVEY

Base Paper 1 - DFT study of adsorption properties of the ammonia on both pristine and Si-doped graphene Nanoflakes.

The overall inference to be taken out from the paper includes Si-doped graphene Nano flakes stated to have higher electrical conductivity and higher sensitivity for the target molecule of Ammonia towards Silicon doped Graphene Nanoflakes than Ammonia towards the pure Pristine Graphene Nanoflakes. No additional research data has been used for the article.

Gas sensing has become a critical area of research due to its significance in environmental monitoring and human health. Ammonia (NH3), a volatile chemical with a low boiling point, poses considerable challenges in the accurate monitoring and control of atmospheric conditions. In response, the scientific community has been actively engaged in developing effective gas-sensitive materials to address this issue.

The emergence of nanotechnology has opened new avenues for the development of gas sensors, with graphene and similar 2D nanomaterials garnering significant attention due to their exceptional mechanical, electronic, and optical properties. Graphene has demonstrated immense potential as an extremely sensitive gas sensor, owing to its high surface area-to-volume ratio and capacity for adsorption.

To overcome these limitations, researchers have explored various strategies, including Nano-structuring graphene into graphene nanoflakes (GNFs), graphene nanoribbons (GNRs), and carbon nanotubes (CNTs), as well as chemical functionality. Graphene nanoflakes, resulting from Graphene's quantum confinement, offer controlled band gaps, making them promising candidates for graphene-based applications.

The excellent electrical properties and structure of GNFs have stimulated considerable interest in their application as physical transducers in gas sensors, promising higher performance in sensitivity and selectivity compared to other diagnostic devices.

Theoretical investigations into nanostructures like Si-doped graphene have intensified in recent years, aiming to expand their utility as nano-catalysts for catalytic reactions and gain deeper insights into their properties for gas sensing applications.

Experimental studies have also demonstrated the efficiency of doping in enhancing stability and catalytic activity, with Si-doped graphene showing promising results in adsorbing NH3 molecules.

In this context, the present study contributes to the understanding of molecular interactions at the nanoscale by employing density functional theory (DFT) calculations to evaluate the adsorption properties of NH3 molecules on pristine and Si-doped graphene nanoflakes.

The study highlights the significant enhancement in NH3 chemisorption onto Si-doped graphene nanoflakes, indicating their potential as effective nano-sensors for NH3 detection.

Overall, the literature survey underscores the importance of exploring nanomaterials, particularly Si-doped graphene, for gas sensing applications, offering valuable insights into the design and optimization of nano-sensors for environmental monitoring and human health protection.

Base Paper 2 - DFT study of NH3(H2O) n=0,1,2,3 complex adsorptions on the (8, 0) single-walled carbon nanotube.

Carbon nanotubes (CNTs) have garnered substantial interest since their discovery in 1991 due to their unique properties and potential applications. Among the diverse investigations surrounding CNTs, understanding their interaction with gases, particularly ammonia (NH3), has been a focal point. NH3 adsorption on single-walled carbon nanotubes (SWCNTs) presents intriguing challenges and opportunities, especially considering the sensitivity of SWCNTs to gaseous molecules. While the interaction is primarily governed by dispersion forces, the presence of NH3's permanent dipole moment introduces additional complexities, influencing dipole-induced dipole and dipole-quadrupole interactions.

A recent theoretical endeavor delves into the adsorption behaviour of NH3 and NH3(H2O) n=1,2,3 complexes on (8, 0) carbon nanotubes, employing density functional theory (DFT) calculations. This study elucidates the intricate nature of the tube-NH3 interaction by exploring parameters such as binding energy (EB), coupling energy (EC), charge density, molecular orbitals, and dipole moments. The findings shed light on how the addition of water molecules to the NH3-tube system enhances the interaction between the tube and NH3 molecule.

In summary, investigations into NH3 adsorption on CNTs not only deepen our understanding of fundamental interactions but also hold promise for various applications, including chemical sensing and gas separation. The study contributes valuable insights into this complex interplay, paving the way for further advancements in this field.

CHAPTER III

COMPUTATIONAL DETAILS

Carbon Nanotube initially was built with the QuantumATK Software. The principle behind CNT includes exhibiting excellent electrical, thermal and mechanical properties. They have been extensively studied for their potential use in sensors, transistors, and interconnects due to their exceptional conductivity and quantum mechanical behaviour.

CNT is primarily a tube made of Carbon atoms with its diameter in a nano-scaled regime.

Both Prominent types of carbon nanotubes include the Single-Walled carbon nanotube and multi-walled nanotube (SWCNT & MWCNT).

The design of CNT is made using the Builder tool, one of the major and an essential tool to give rise to building the desired molecule structures from the elements available in the database. A hexagonal line up of Carbon atoms with double bonds forms a Graphene which when folded will be a single-walled carbon nanotube - SWCNT.

Nested layers of a single-walled carbon nanotube give rise to the multi-walled carbon nanotube. Double bonding between the Carbon atoms and nano-scaled factor helps in tensile strength and conductivity. Co-vaporizing Carbon and the transition metals catalyze SWCNT formation led to an increase in research of applications and characterize SWCNTs.

The two arrangements for CNTs are Armchair and Zigzag inclusive of infinite nanotube cylindrical in structure. The discovery of the Carbon Nanotube involves Graphite taken as two electrodes and when current is passed through, a cloud of carbon gases begins to create vaporizing the tip of the anode rod.

Small-layered threads of Carbon were observed which is CNT, the most tensile element known to mankind. Apart from using it to sense gases, different types of field effect transistors were also possible to be built.

QuantumATK

The collaboration of academic researchers and computer professionals made it possible to set up the first-ever nano-scale modelling tools being integrated as a set forming QuantumATK Software. The device simulation algorithm based on DFT (density

functional theory) is a lot faster since it is built from the ground to provide maximum accuracy.

Steps involved for Computational purposes:

• Builder Tool

Availability of Carbon Nanotube from the database of software to design.

 Create the structure of CNT configured using the value of number of layers, atoms, lattice length, surface cleave and atomic coordinates using the advanced building tools in QuantumATK Builder.

 Initially, a new project is to be created and to be directed to the design window.
Usage of the Builder Database is done by importing the Nanotube structure. Atomic coordinates are changed according to the cell dimensions measured in the nanoscale.

 Surface-Cleave, a plugin is used to create the formatted nanotube along with the vacuum surrounding it. Furthermore, more atoms or molecules are added with the use of a database at the required position. Usually, the magnitude of lattice vectors is increased.

 The plugin plays a major role in deciding whether to form the structure as a periodic or a non-periodic and normal slab type. The configuration built once completed was sent to the Stash.

• Script Generator Tool

 The Selection tool is present to ensure no overlapping between the atoms bound to be present to prevent undesired change in the electronic properties. After finishing with the build of CNT, the molecule is sent to the Script Generator. Data Calculation for the given design is made with the tools and the software provides a. hdf5 file consisting of storage for the logs related to analyzed properties.

 Script Generator involves the manipulation of parameters to construct the existing potential of the Carbon elements which are present in the Nanotube. The parameters are modified using the two tool elements present in QuantumATK -- Calculator & Optimization.

 Using isotope doping, thermoelectric-related effects of Carbon Nanotubes.

 In the CNT, different isotopes have significant marks on their properties. The known factor is that the mass of the nucleus doesn't have any effect on its electronic properties. But having changed to its isotopes makes a greater impact.

 Under the tool, three blocks consisting of a New Calculator, Density of States, and total energy were added. A New Calculator was referred to set the K-point sampling with differential constants, and to gain more speed in analyzing the properties the exchange correlation was reduced to Single-zeta polarization.

 The Density of the States block consisted of parameters including K-point sampling, the range of energy in eV, and the number of sample points. DoS contains all information about the density state of the device region.

 Both the textual representation and the two-dimensional plot for both total energy and density of states once ready is accessed through the main channel for output. A script will then be generated which is to be sent to the Job Manager to execute them.

• Job Manager Tool

All the logs and the data to be run occur behind the screen with the strong computational DFT Simulation based algorithm taking place. In the Lab-Floor the files will be attached once the jobs get compiled one at a time.

• Viewer Tool

Once calculation is over, the. The hdf5 file will be marked with a completed symbol under the files of project. Report in the form of objects is now visible for the users to fetch the results.

- **Editor Tool**

During building and segregating the parameters to satisfy the electronic properties, editor tool comes in handy if in case the computational steps involved is taken care of with any minor error till the structural level.

CHAPTER IV

RESULTS

4.1 Design using Viewer tool

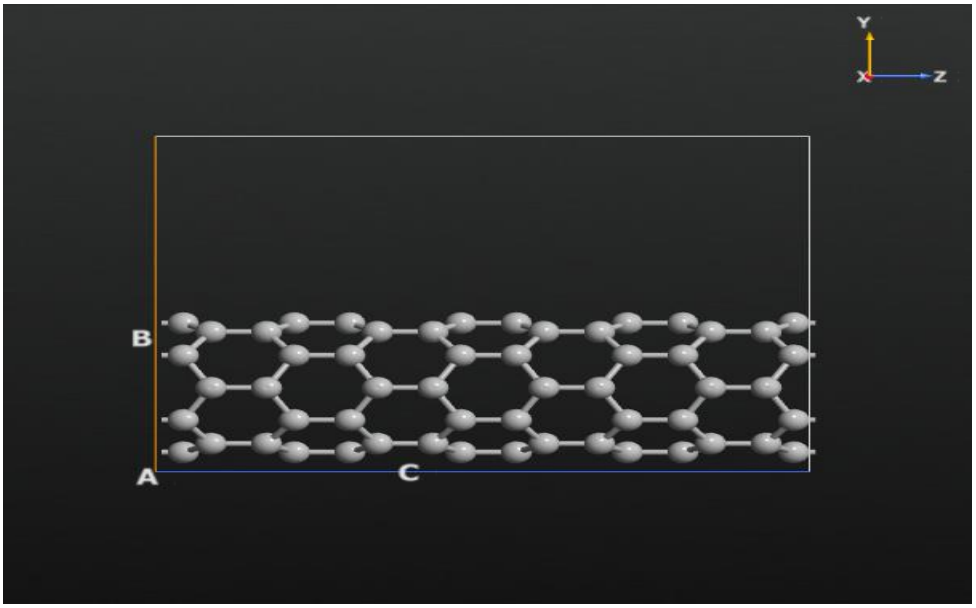

Fig .2 Carbon Nanotube

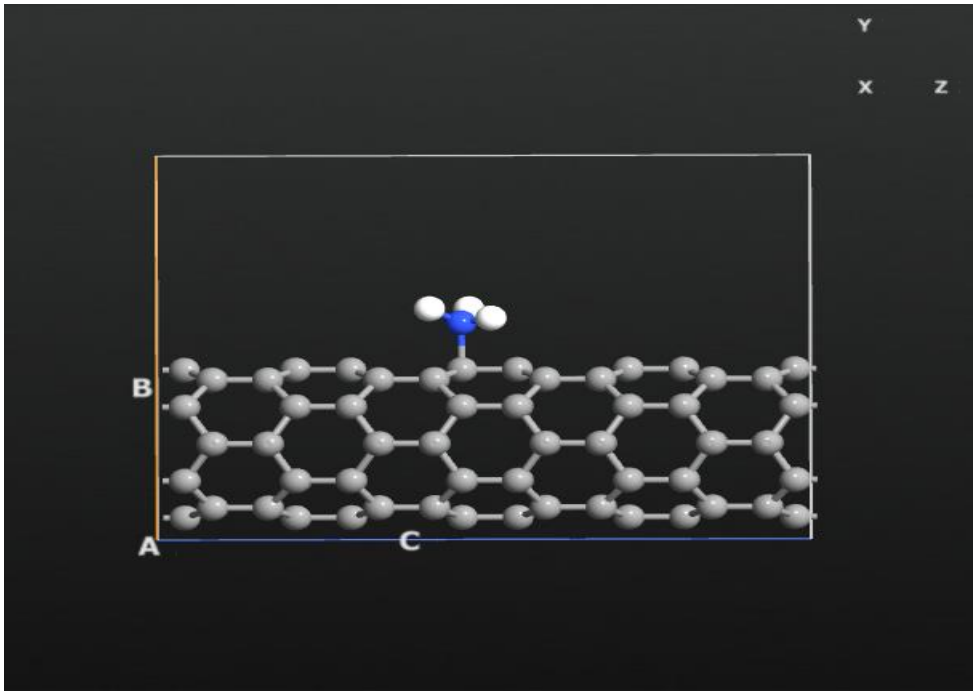

Fig 3 Carbon Nanotube doped with Ammonia

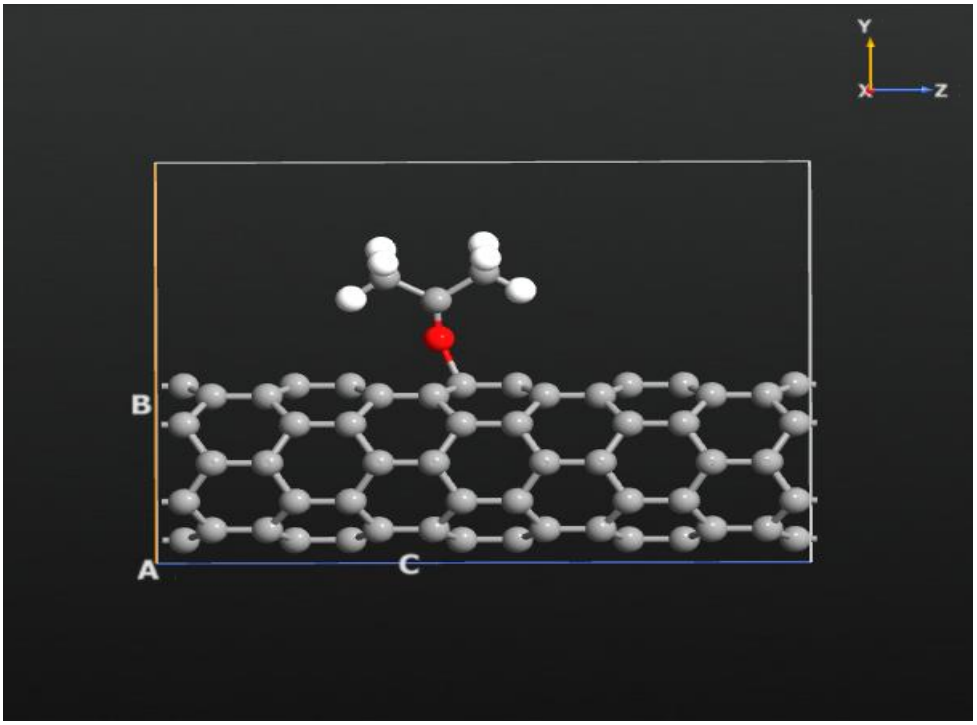

Fig 4 Carbon Nanotube doped with Acetone

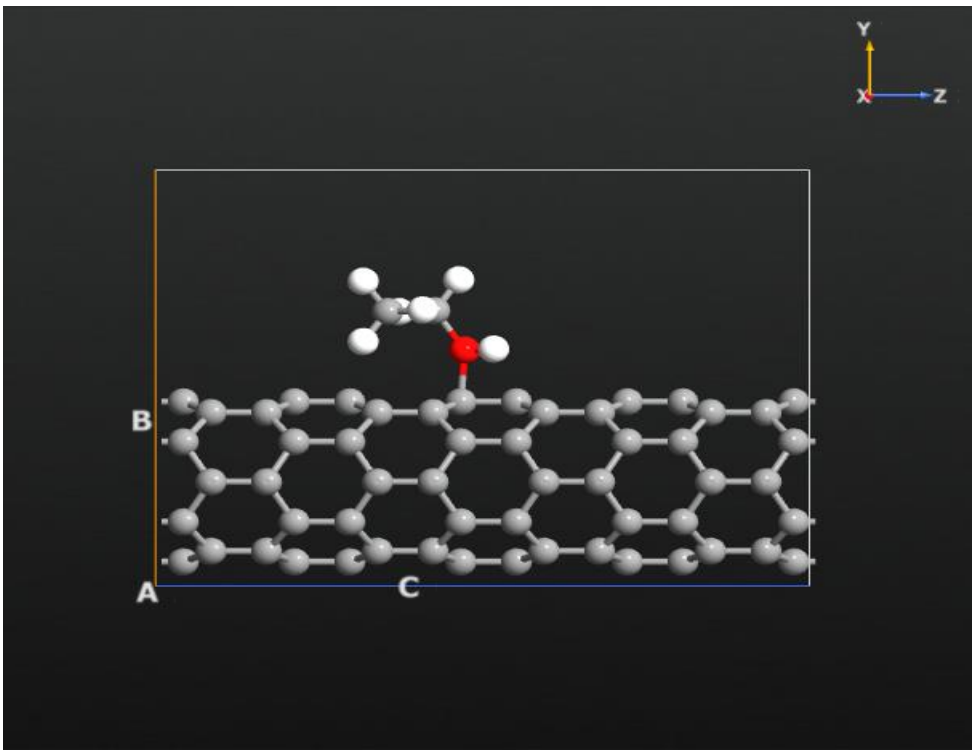

Fig .5 Carbon Nanotube doped with Ethanol

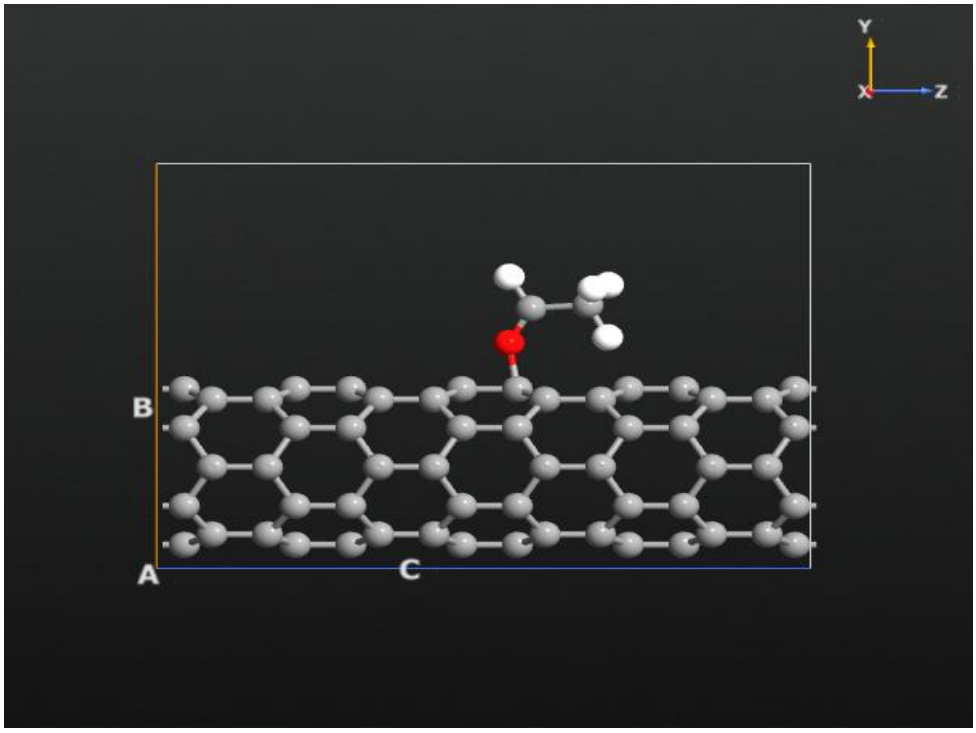

Fig .6 Carbon Nanotube doped with Ethanal

4.2 Total Energy Report

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| Total Energy Analysis                                                         |
|                                                                               |
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| External-Field                  =    0.00000 eV                               |
| Exchange-Correlation            = -5030.11937 eV                              |
| Kinetic                         =  10961.57946 eV                             |
| Electrostatic                   = -20958.20074 eV                             |
| Entropy-Term                    =   -0.04649 eV                               |
+-------------------------------------------------------------------------------+
| Total energy                    = -15026.78714 eV                             |
+-------------------------------------------------------------------------------+
```

Fig .7 Carbon Nanotube

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| Total Energy Analysis                                                       |
|                                                                             |
+-----------------------------------------------------------------------------+
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| Kinetic                           =  11219.17806 eV                          |
| Electrostatic                     = -21425.75695 eV                          |
| Entropy-Term                      =   -0.06825 eV                            |
+-----------------------------------------------------------------------------+
| Total energy                      = -15344.18944 eV                          |
+-----------------------------------------------------------------------------+
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Fig .8 Carbon Nanotube doped with Ammonia

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|                                                                             |
| Total Energy Analysis                                                       |
|                                                                             |
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| External-Field                    =    0.00000 eV                           |
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| Kinetic                           =  11695.57615 eV                          |
| Electrostatic                     = -22380.23034 eV                          |
| Entropy-Term                      =   -0.05522 eV                            |
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Fig .9 Carbon Nanotube doped with Acetone

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| Total Energy Analysis                                                       |
|                                                                             |
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| Kinetic                         =  11596.26860 eV                           |
| Electrostatic                   = -22171.14495 eV                           |
| Entropy-Term                    =   -0.06101 eV                             |
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Fig .10 Carbon Nanotube doped with Ethanol

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| Total Energy Analysis                                                       |
|                                                                             |
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| Exchange-Correlation            = -5030.11937 eV                            |
| Kinetic                         =  10961.57946 eV                           |
| Electrostatic                   = -20958.20074 eV                           |
| Entropy-Term                    =   -0.04649 eV                             |
+-----------------------------------------------------------------------------+
| Total energy                    = -15026.78714 eV                           |
+-----------------------------------------------------------------------------+
```

Fig .11 Carbon Nanotube doped with Ethanal

4.3 Density of States

4.3.1 DoS of Carbon Nanotube

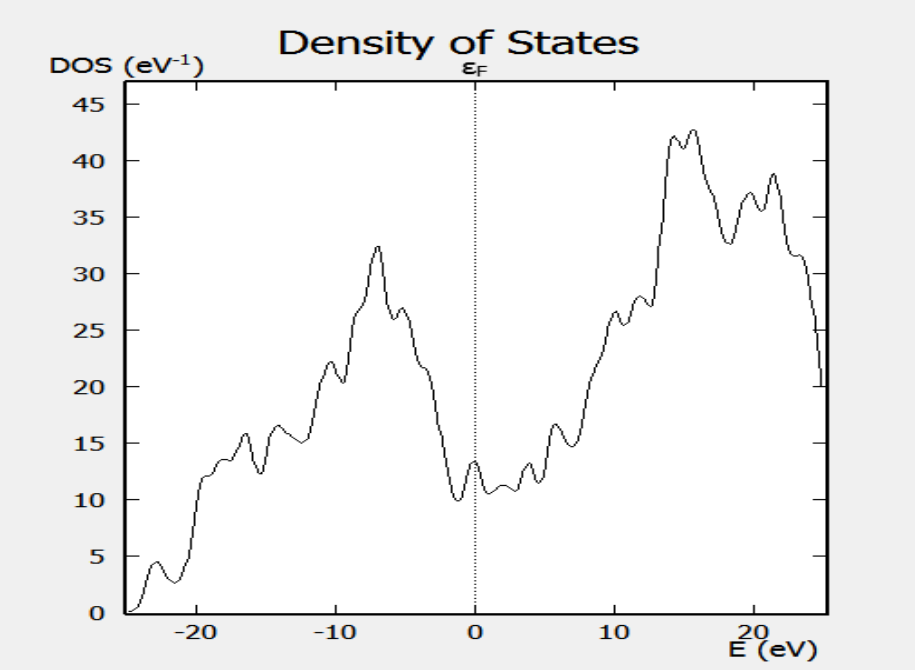

Fig .12 s-, p-, d- orbital electrons

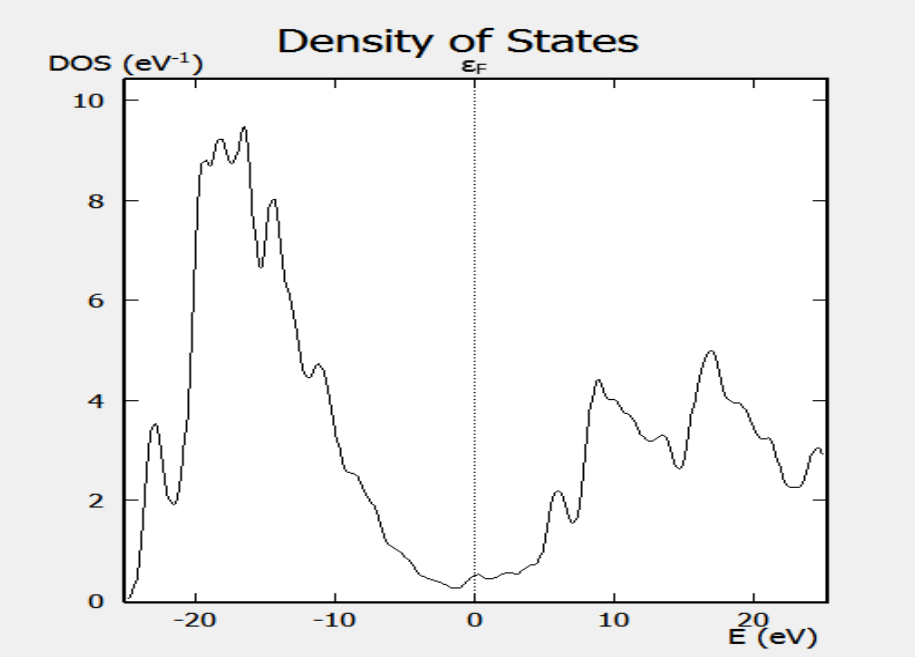

Fig .13 s- orbital electronS

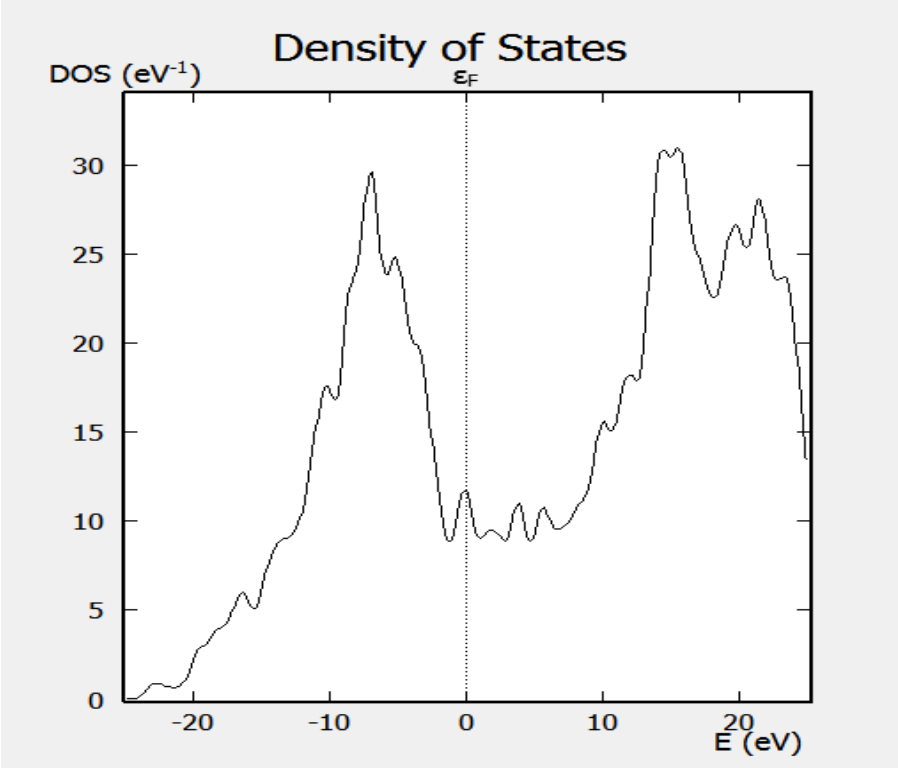

Fig .14 p- orbital electrons

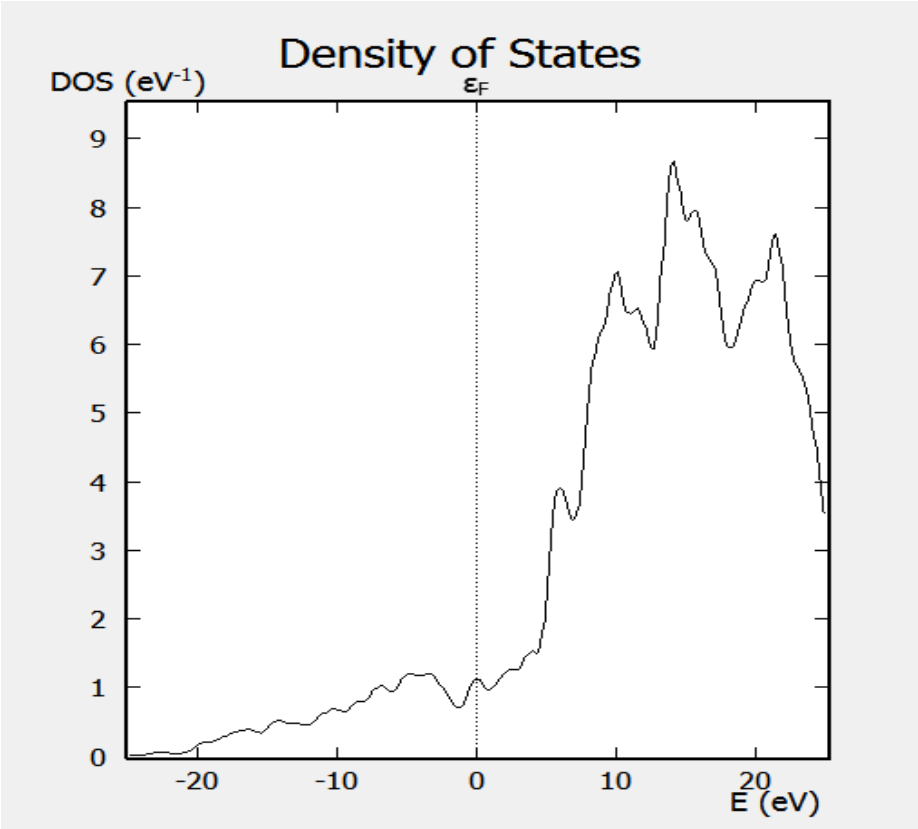

Fig .15 d- orbital electrons

4.3.2 DoS for CNT & Ammonia

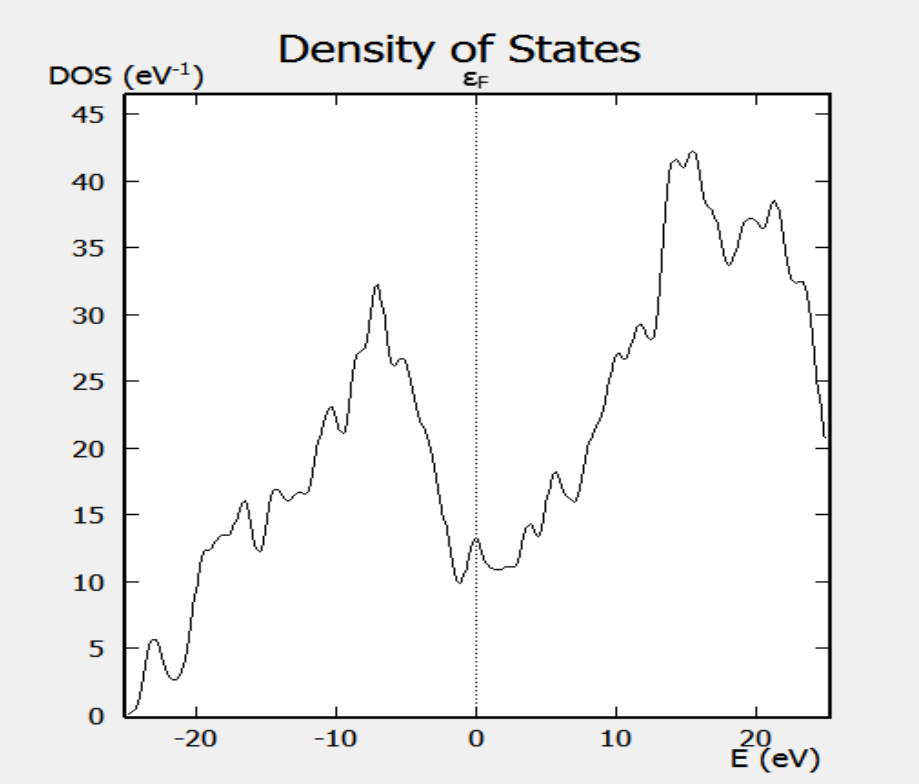

Fig .16 s-, p-, d- orbital electrons

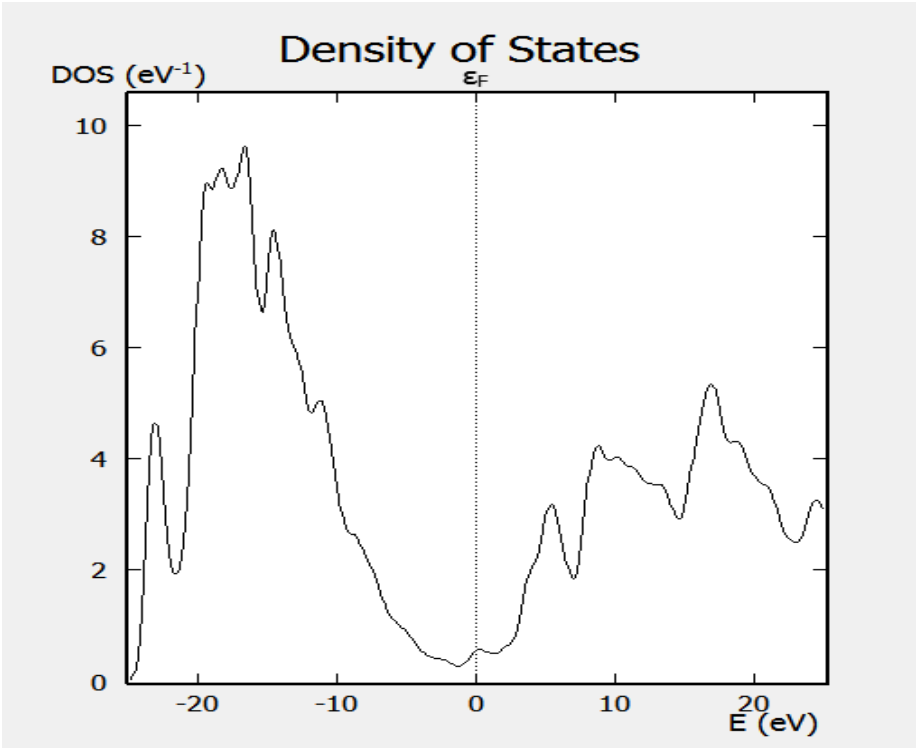

Fig .17 s- orbital electrons

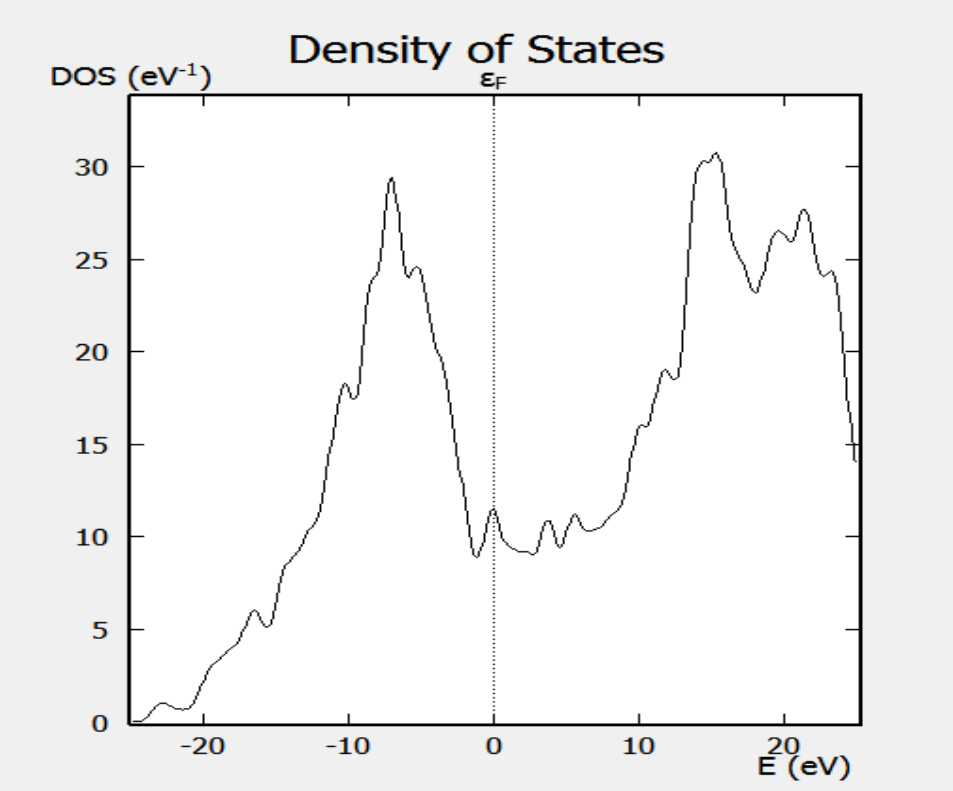

Fig .18 p- orbital electrons

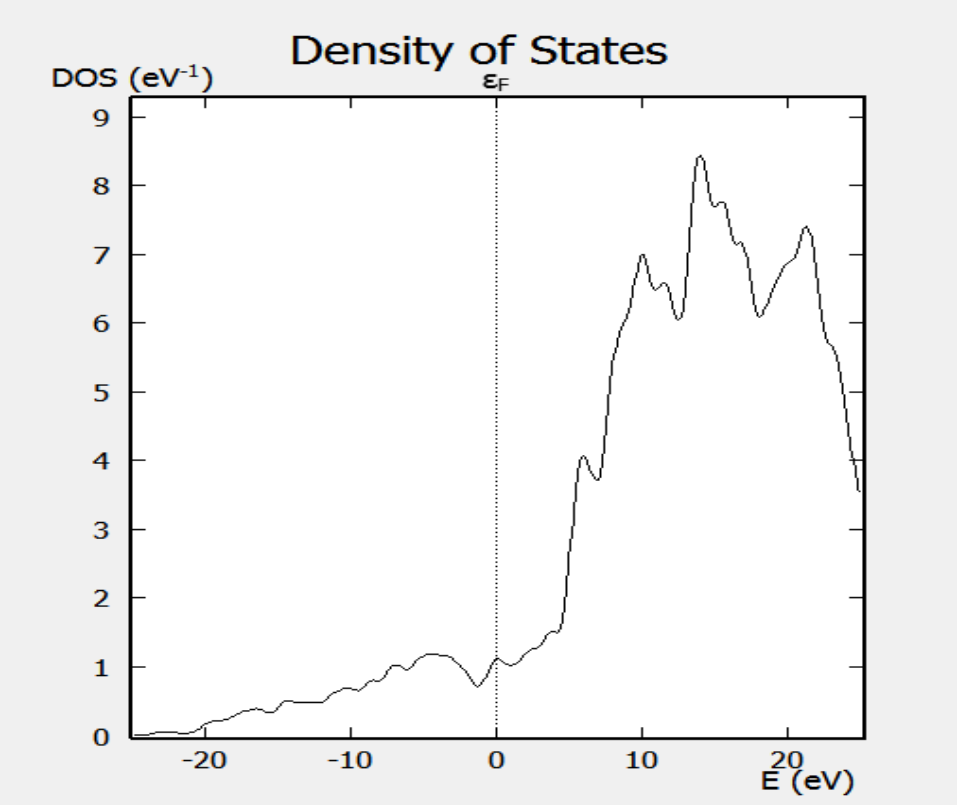

Fig .19 d- orbital electrons

4.3.3 DoS of CNT & Acetone

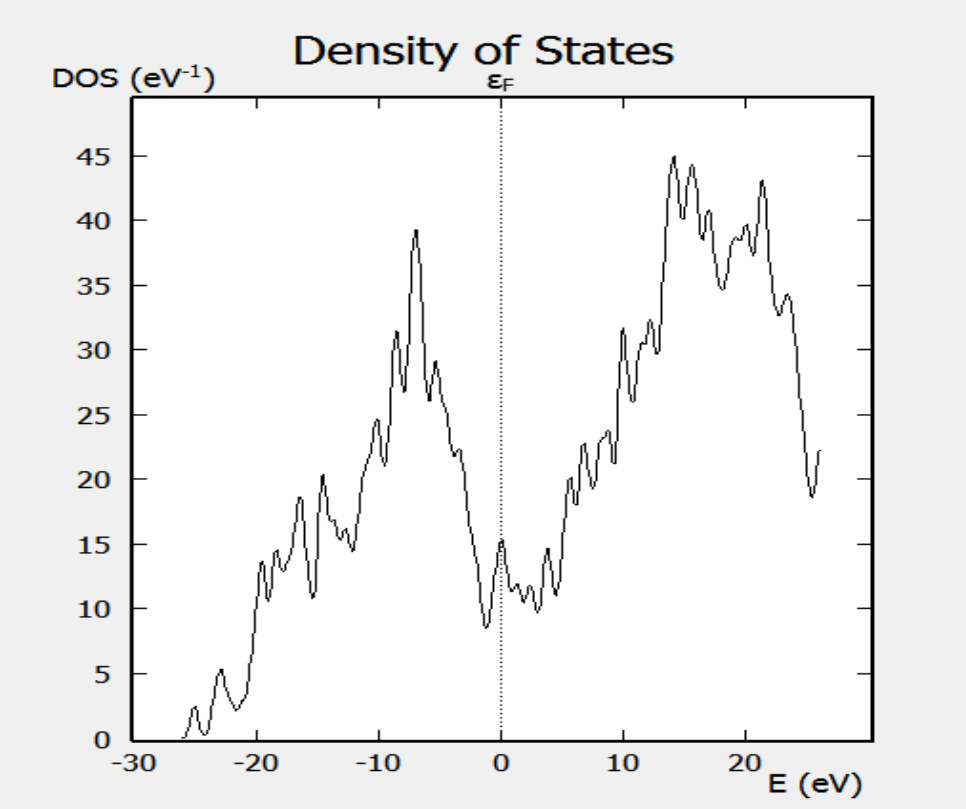

Fig .20 s-, p-, d- orbital electrons

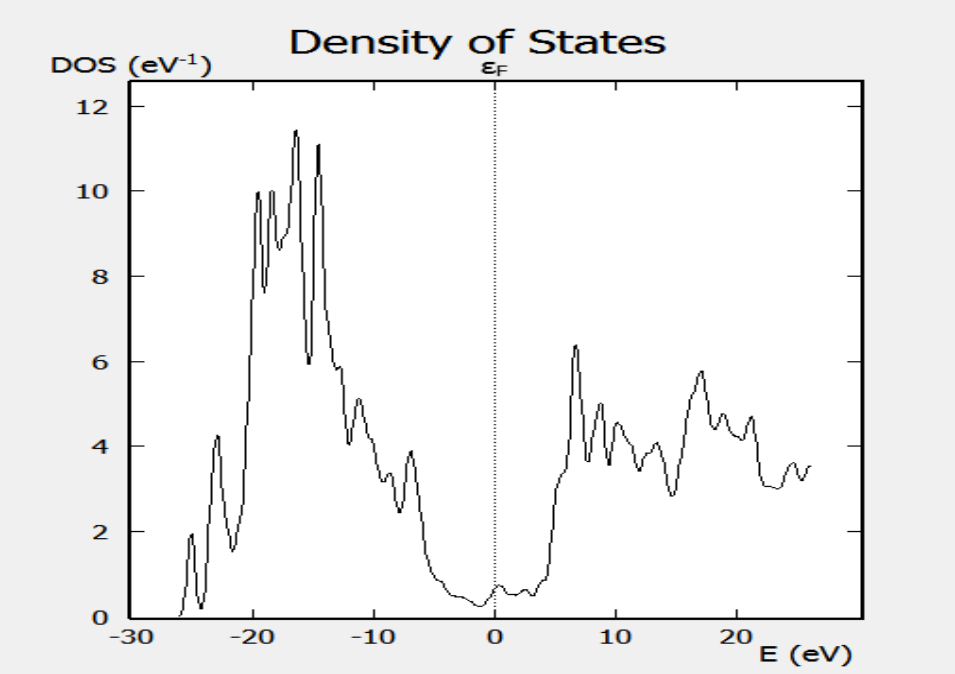

Fig .21 s- orbital electrons

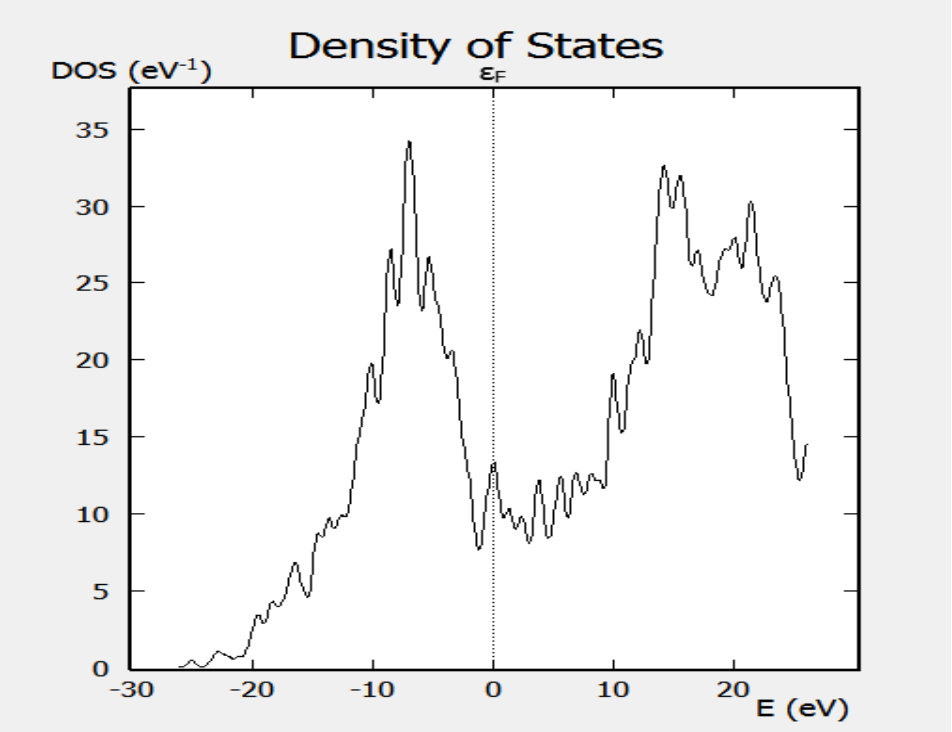

Fig .22 p- orbital electrons

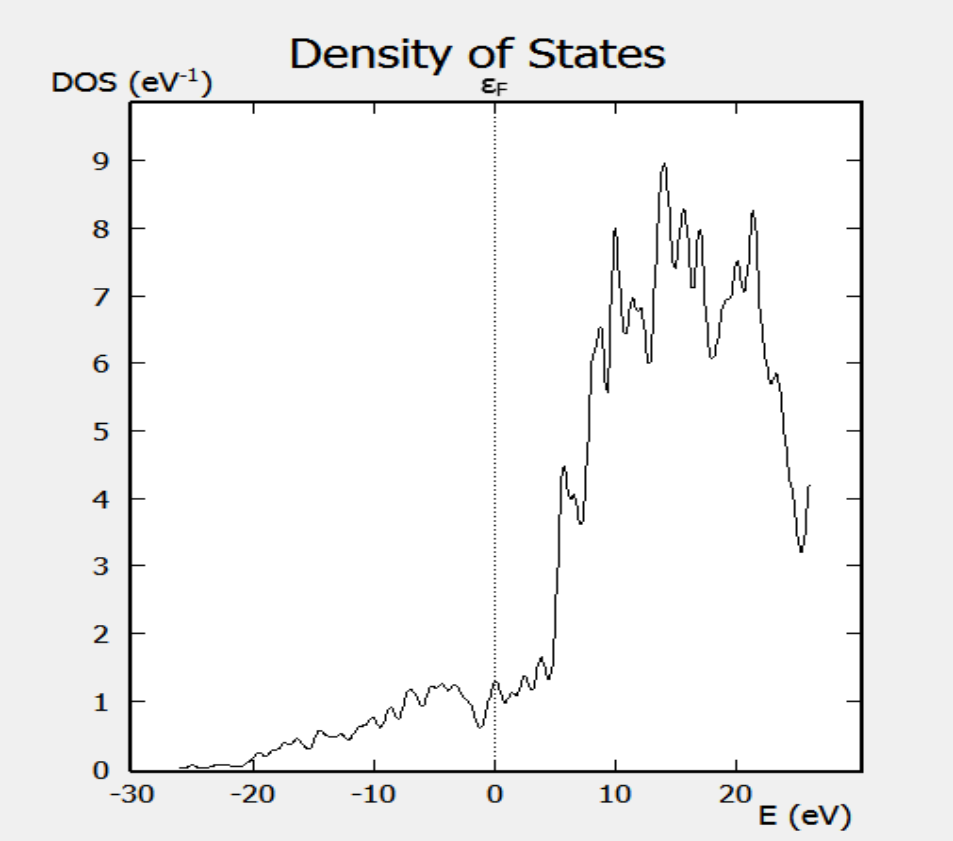

Fig .23 d- orbital electrons

4.3.4 DoS of CNT & Ethanol

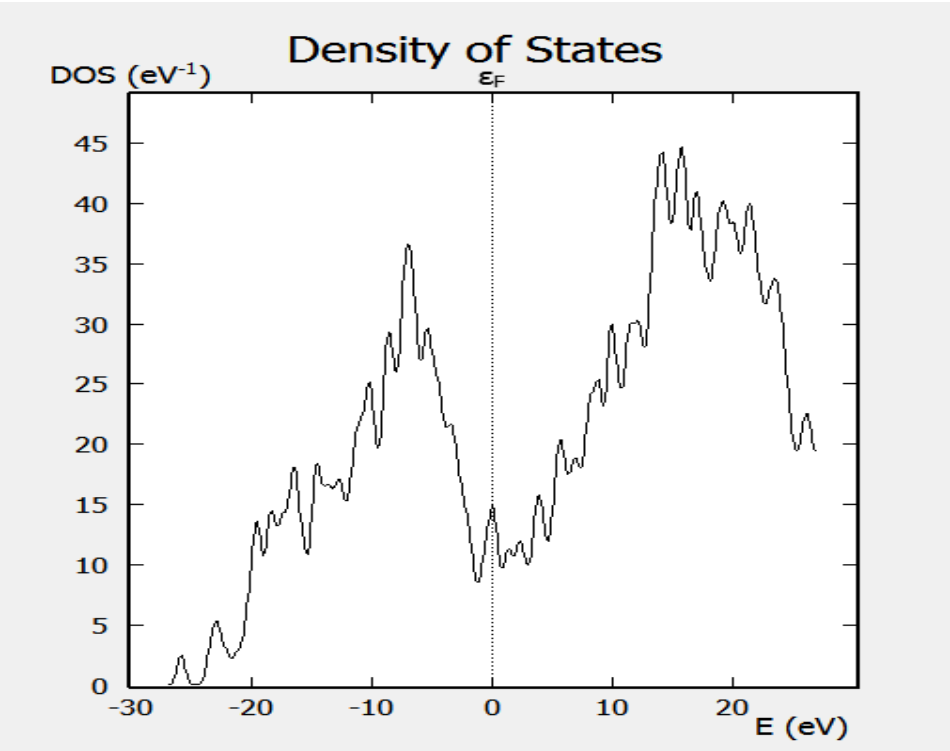

Fig .24 s-, p-, d- orbital electrons

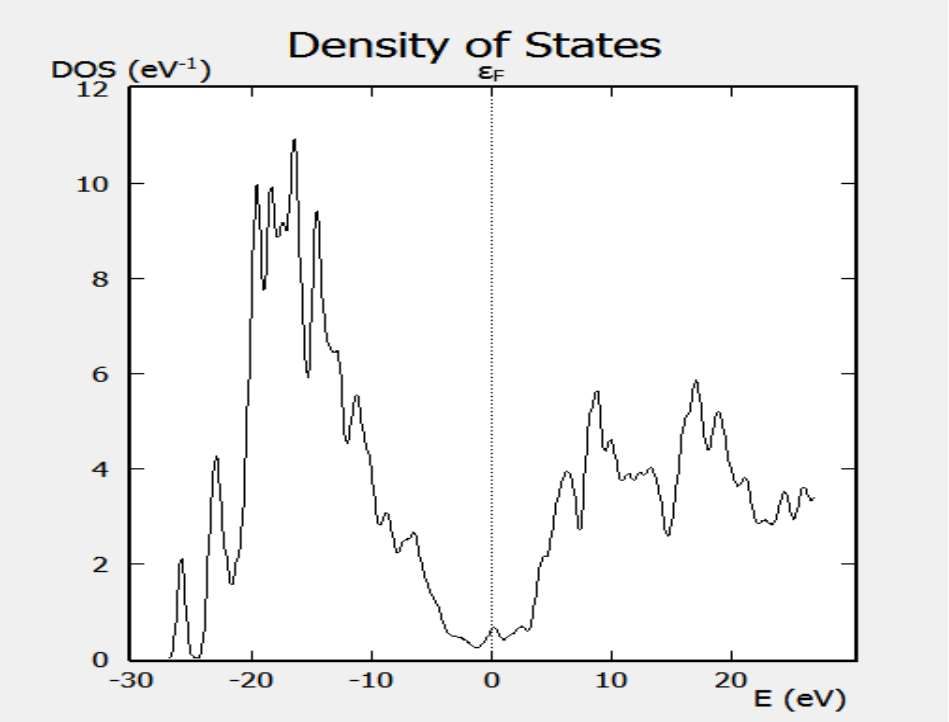

Fig .25 s- orbital electrons

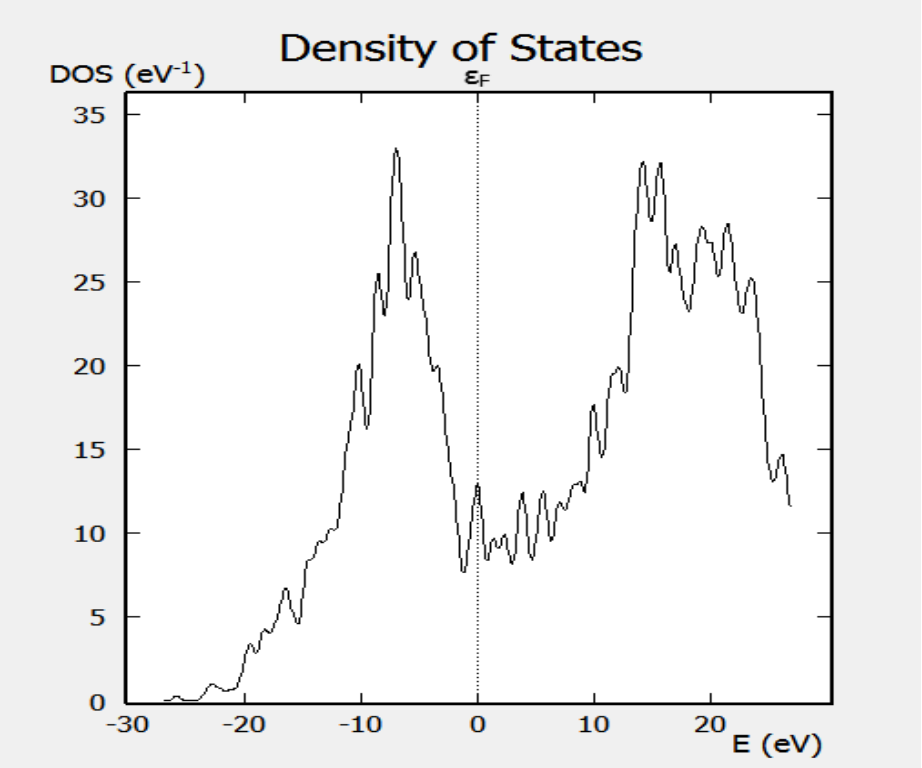

Fig .26 p- orbital electrons

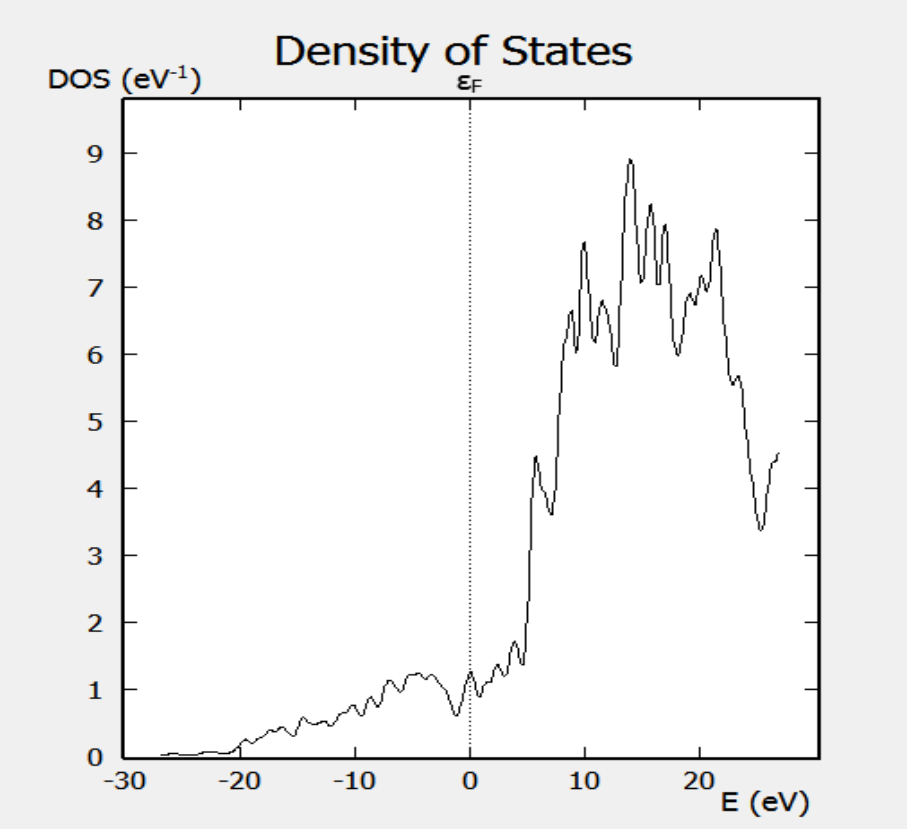

Fig .27 d-orbital electrons

4.3.5 DoS of CNT & Ethanal

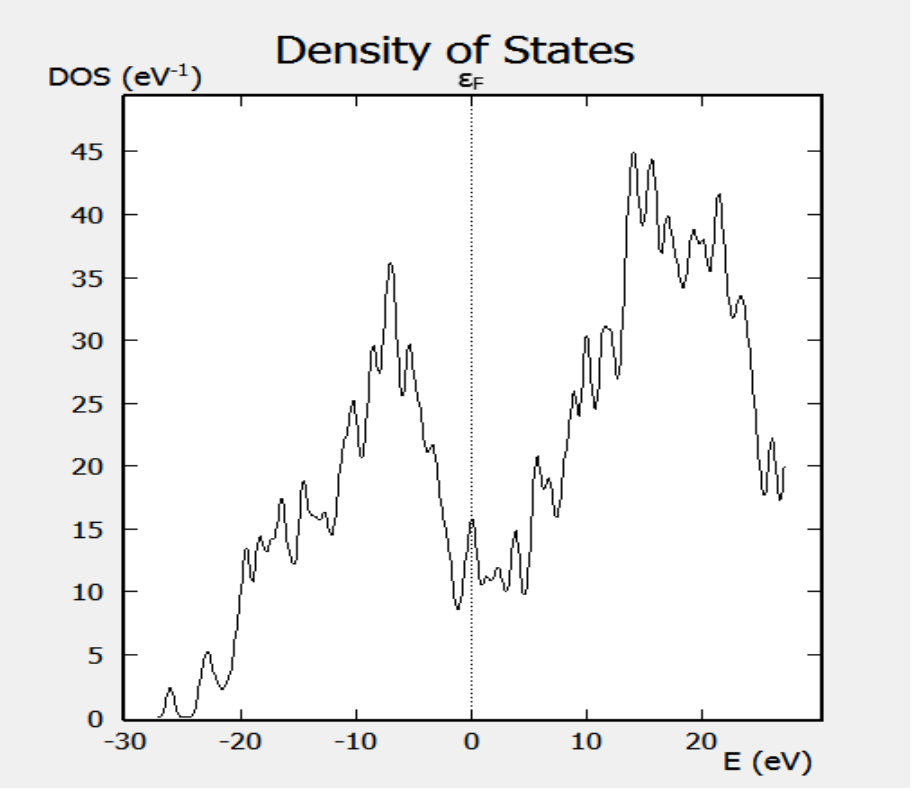

Fig .28 s-, p-, d- orbital electrons

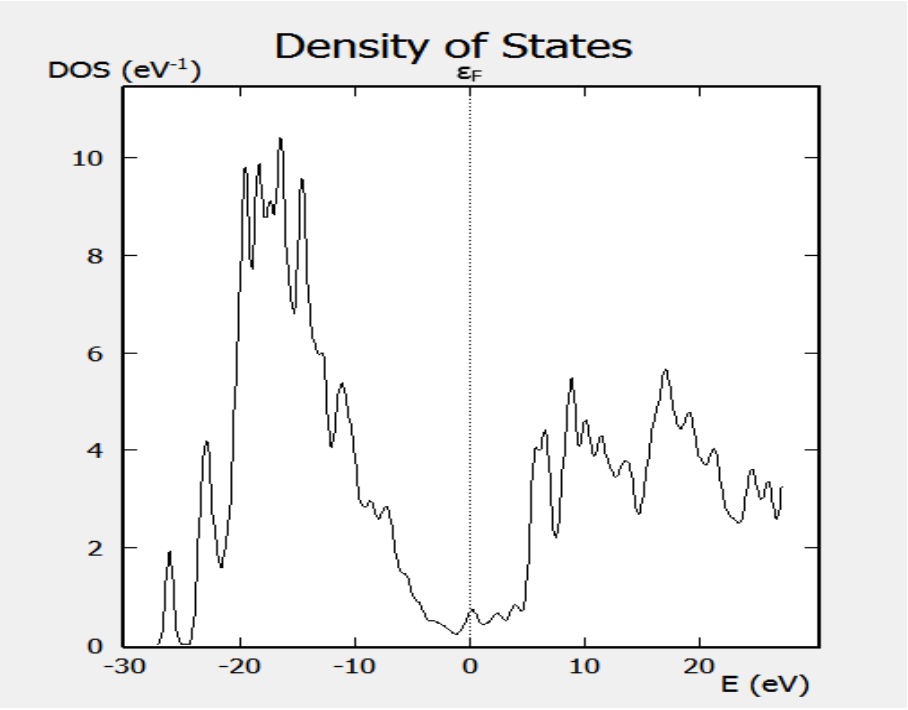

Fig .29 s- orbital electrons

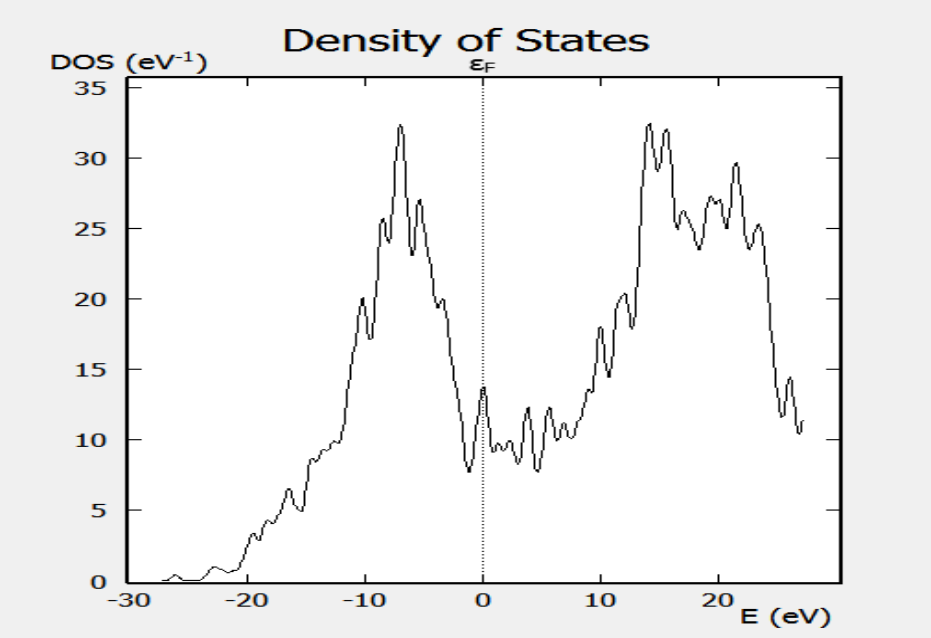

Fig .30 p- orbital electrons

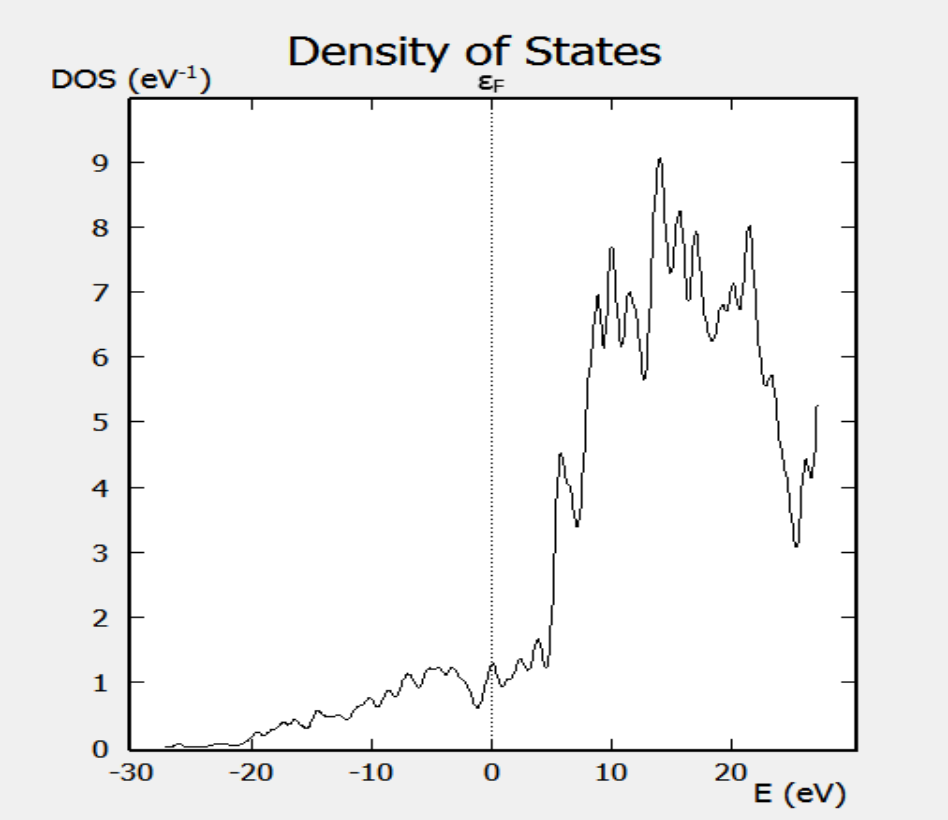

Fig .31 d- orbital electrons

4.4 Compare DoS of CNT

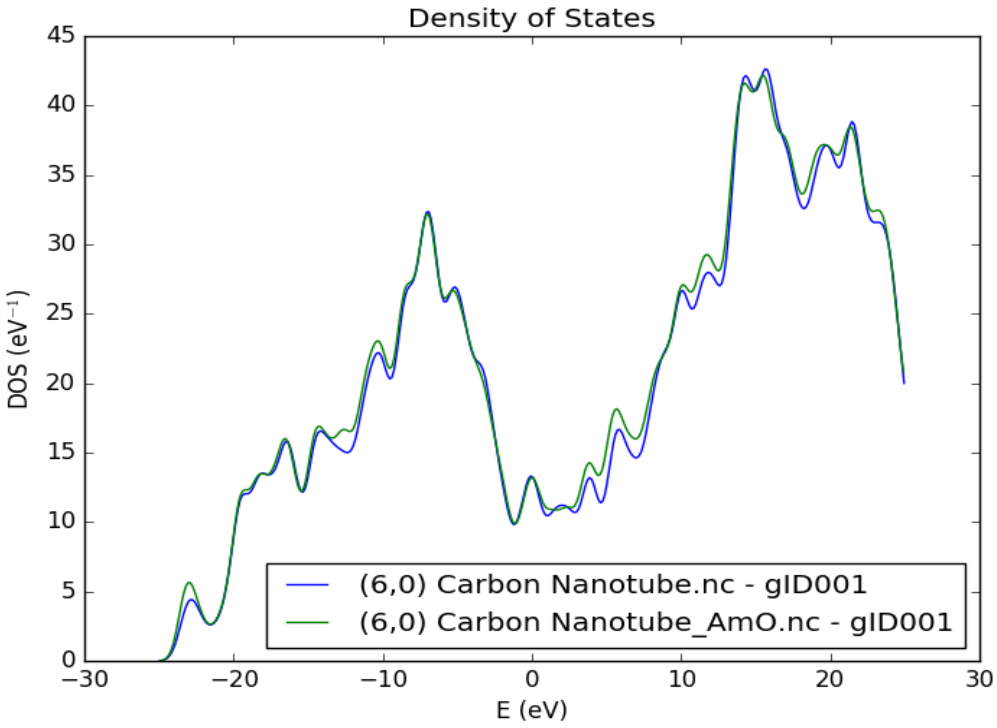

Fig .41 Carbon Nanotube doped with Ammonia

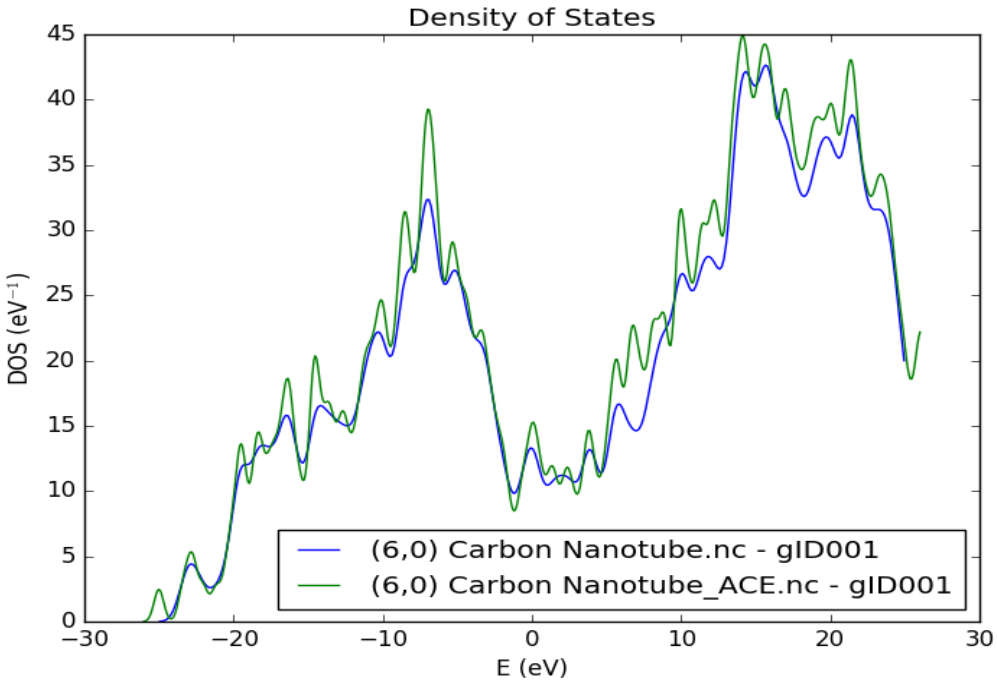

Fig .42 Carbon Nanotube doped with Acetone

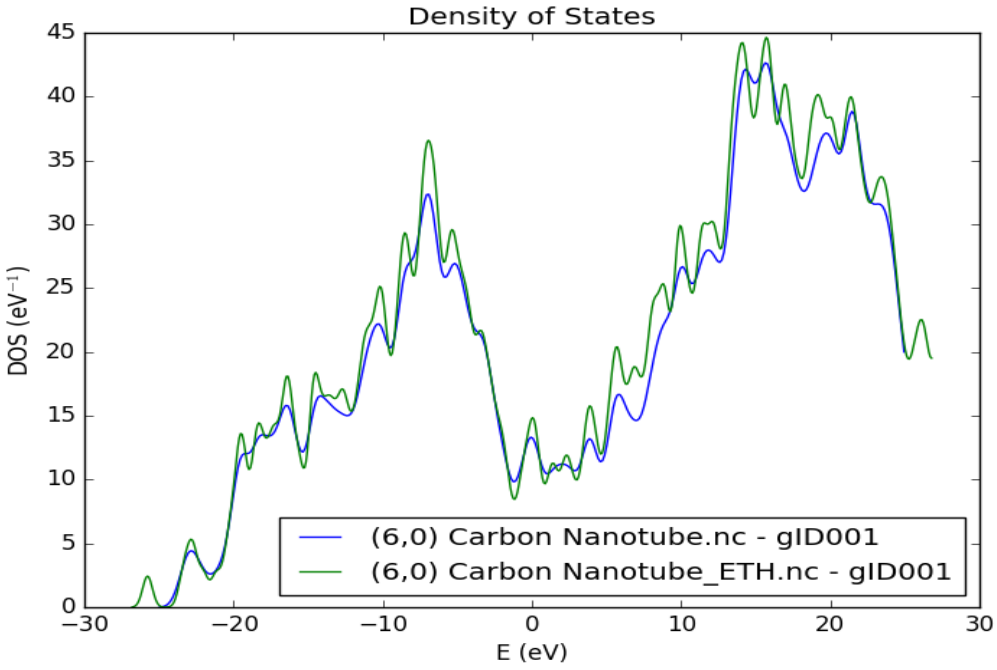

Fig .43 Carbon Nanotube doped with Ethanol

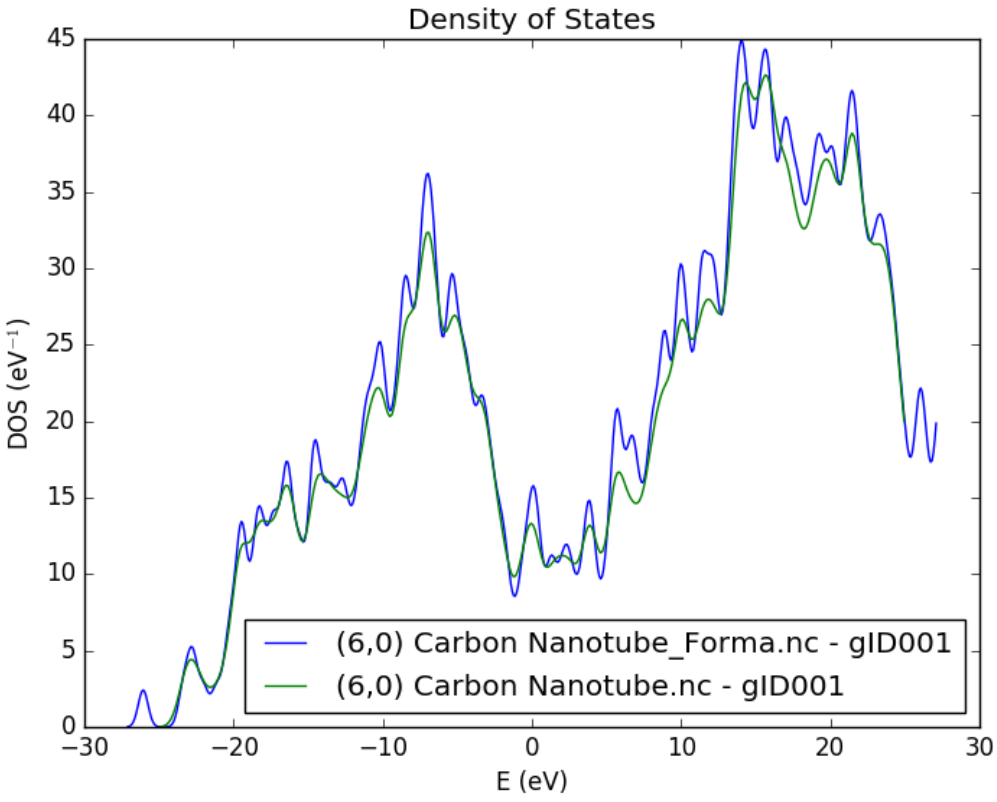

Fig .44 Carbon Nanotube doped with Ethanal

4.5 Compare Carbon Nanotube, target molecule & combined

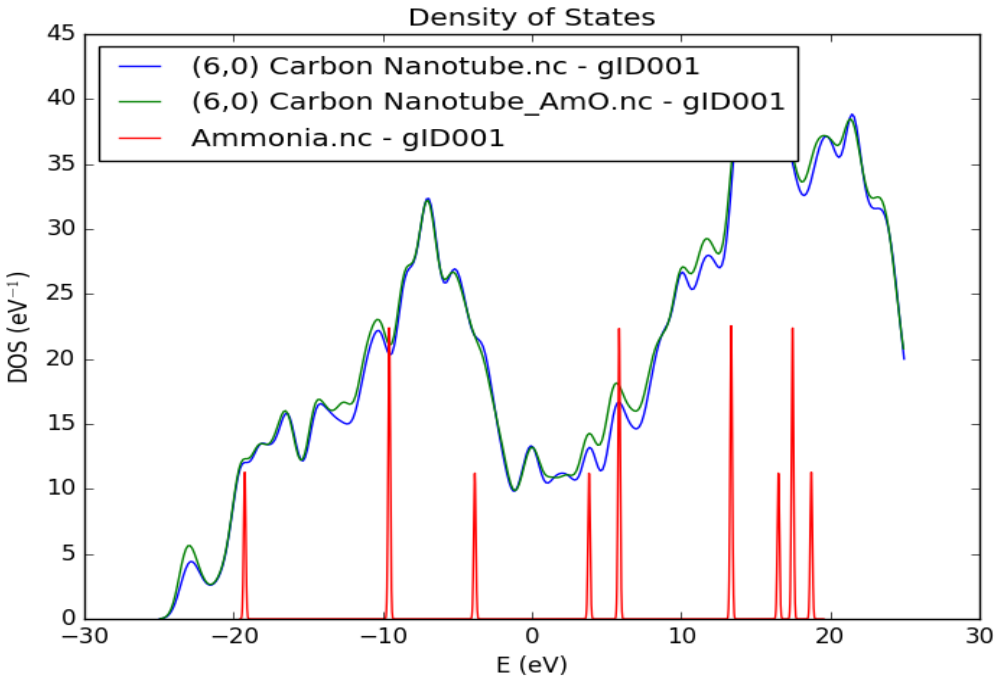

Fig 45 CNT, Ammonia & CNT with Ammonia

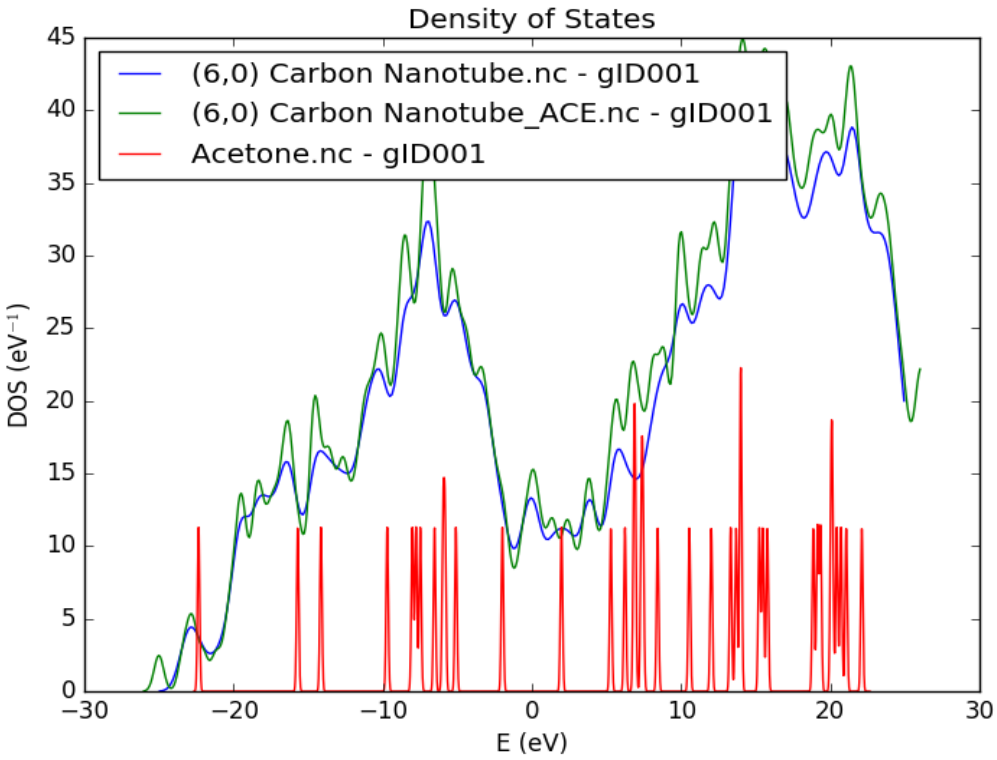

Fig .46 CNT, Acetone & CNT with Acetone

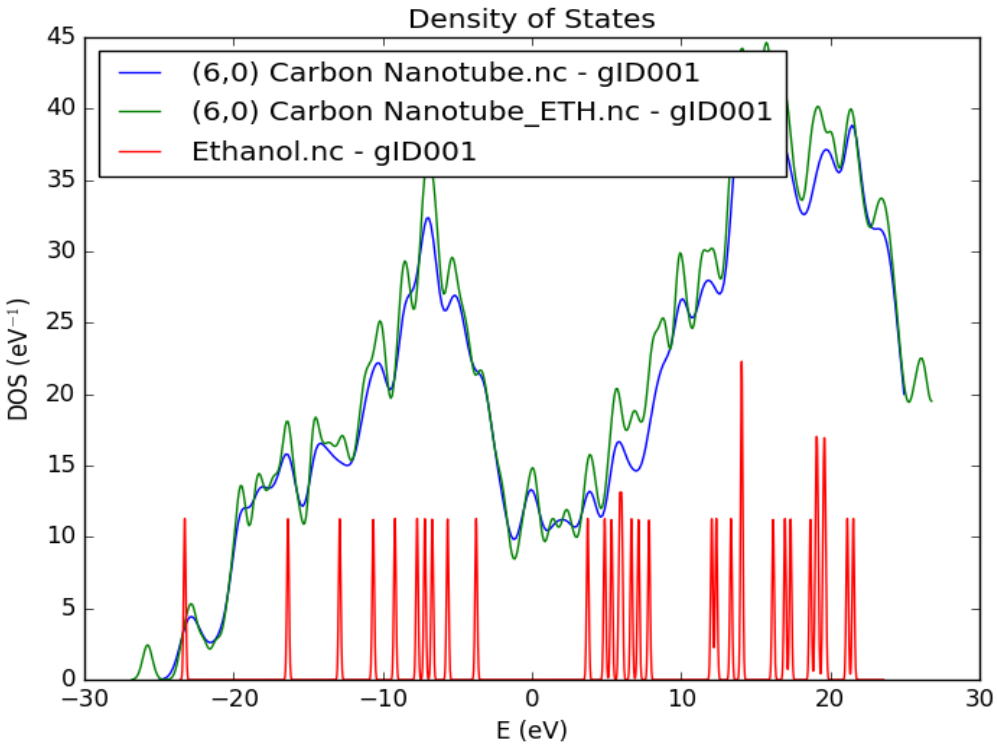

Fig .47 CNT, Ethanol & CNT with Ethanol

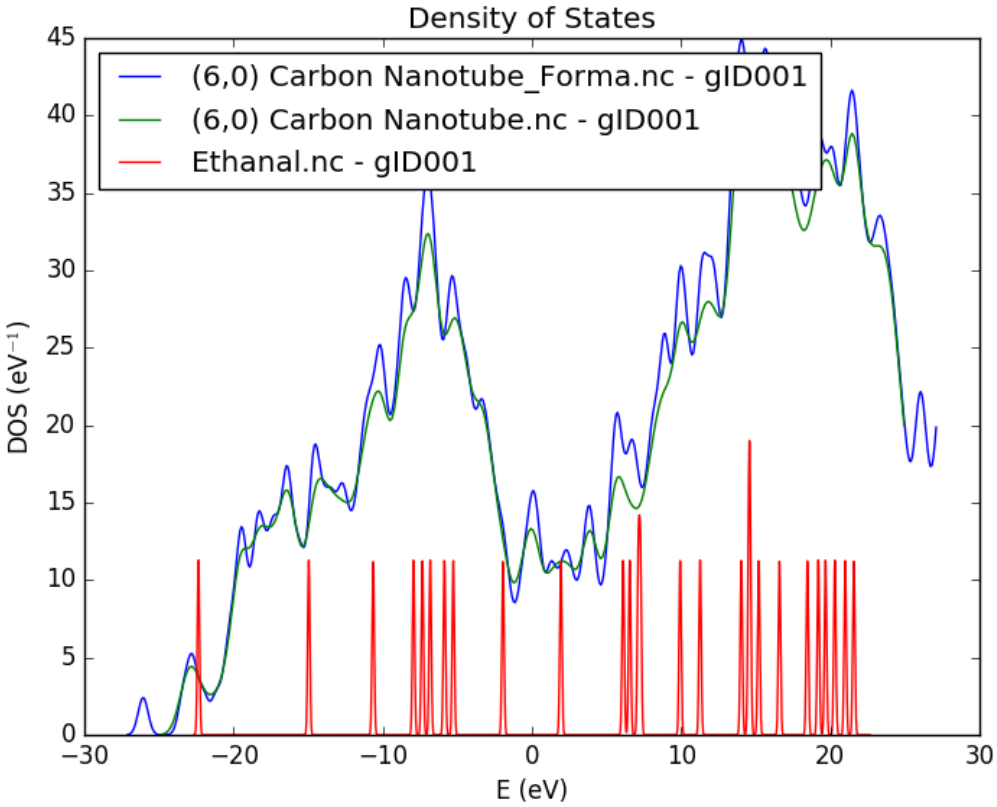

Fig .48 CNT, Ethanal & CNT with Ethanal

CHAPTER 5
CONCLUSION

SUMMARY & FUTURE OUTLOOK

Density functional theory calculation with GGA Approximation was performed to study the electronic properties of carbon nanotubes by analyzing the interaction with the target molecule. Being a promising material to be utilized for gas sensing applications comprised of its huge electrical conductivity, the density functional theory calculations, particularly through the analysis of Density of States (DoS), provide insights into the electronic structure and properties of CNTs and their interaction with gas molecules.

The change of transfer phenomena or in conductivity changes by exploiting it to molecules thereby understanding the distribution of electronic states in CNTs and how they are influenced with the presence of gas molecules.

Future Research will be focusing on engineering the Density of States of CNTs through structural modifications, doping or with functionality to enhance their sensitivity to specific gas molecules. Researchers can optimize the electronic response of CNT based sensors with predictable and tunable characteristics.

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https://doi.org/10.1016/j.chphi.2024.100561

2. Yang Z, Zeng Z, Wang K, Wong SS, Liang W, Zanin M et al (2010) DFT study of NH3(H2O) n=0,1,2,3 complex adsorption on the (8, 0) single-walled carbon nanotube
https://doi.org/10.1016/j.commatsci.2010.02.035

APPENDIX

BASE PAPER

Kareem H. Bardan, Fouad N. Ajeel, Mohammed H. Mohammed, Alaa M. Khudhair, Ali Ben Ahmed, "DFT study of adsorption properties of the ammonia on both pristine and Si-doped graphene nanoflakes"

DOI: https://doi.org/10.1016/j.chphi.2024.100561

KEYWORDS: GNFs, Nanosensor, DFT, Adsorption, NH3 molecule.

URL: https://linkinghub.elsevier.com/retrieve/pii/S2667022424001051