

# A Theoretical Study on Lithium Storage Capability of (10, 0) Zigzag Carbon Nanotube

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## ABSTRACT

We studied the Lithium storage capability of (10, 0) zigzag carbon Nanotubes by using *Ab initio* calculations. The main motivation is to use single walled carbon Nanotubes (SWCNTs) to store lithium atoms. By using first principles calculations, the storage of Lithium atoms on the CNT has been studied by considering both inside and outside cases. The band structure, density of states, electron density and was performed by inserting Li atoms. The binding energies are also calculated. We observed that the adsorption of lithium atoms on the outside of the CNT is favored in contrast to the inside.

**Keywords:** *Ab-initio study, Lithium storage, single-walled carbon Nanotubes.*

## I. INTRODUCTION

Since the discovery of Carbon Nanotubes (CNTs) by S.Iijima [1] in 1991, it received much attention irrespective of the technological fields. This is because of their marvelous mechanical and electric properties [2-5]. The theoretical studies [3] predicted that CNTs has very high young's modulus and the same confirmed in experimental studies also [4]. The excellent properties made this useful for wide range of applications. Broadly CNTs can be divided into Single Walled Carbon Nanotubes (SWCNTs) which can be visualized as a grapheme sheet coiled up into a seamless cylinder and Multi Walled Carbon Nanotubes (MWCNTs) consists of numerous rolled layers (concentric tubes) of grapheme. The diameter and length of the nanotube unit cell are defined solely in terms of the Hamada indices and this also dictates the conductivity of the nanotube [5]. Depending up on the chirality and angle of rolled up sheet, CNTs can either be in zigzag or Armchair arrangement. All Armchair (n=m) CNTs are invariably metallic, while zigzag (n, 0) CNTs can be metallic or semiconducting depending up on the diameter.

Recently, the insertion of lithium into carbon nanotubes has drawn much attention. This is because of possible applications as anodes in Li-ion batteries. Several theoretical studies have presented to understand the Lithium storage in single walled carbon Nanotubes (SWCNTs). The absorption energy of Li in CNTs and local Li-C and C-C bonds are investigated by Liu et al. in 2004 by using the first principles calculations. The interaction and concerted diffusion of Li in (5, 5) CNTs was studied by Ehantha et al. using first principles calculations. The results specify that inside CNTs, Li atoms are stable.

In this study, we investigated the behavior of the (10, 0) SWCNT by considering the lithium atoms both inside and outside.

### II. COMPUTATIONAL DETAILS

The Band structure, Density of states and Mulliken population analysis was computed using density functional theory based approach with Non equilibrium green's function (NEGF) [7-8] framework applied through ATK-VNL [6], an Ab initio code, which is a further development of TRANSIESTA-C code. The geometry optimization has been performed using generalized gradient approximation (GGA) as exchange correlation function with Revised Perdew Burke Ernzerhoff (RPBE) type parameterization [9-10]. In order to obtain the total energy convergence, throughout the calculations a large plane wave mesh cut off of 75 Hartree is used with 1x1x20 k-point. Double  $\xi$  polarized basis set with non-local norm conserving pseudo potential was used for elucidate the valance band. The full course optimization was performed.

### III. RESULTS AND DISCUSSION

Lithium is a Group 1 (1A) element having a single valence electron ( $1s^2 2s^1$ ). Group 1 elements are called "alkali metals". It is available in solid only about half as dense as water and it is the least dense metal. Its chemistry is influenced by its trend to lose an electron to form  $Li^+$ . Hence it is a perfect material for batteries. As the lightest metal on the periodic table, it is able to achieve high energy densities by insinuating itself into other materials through a process called "intercalation".

In this paper we performed calculations on (10, 0) zigzag type CNT model. The (10, 0) SWCNT with 79 carbon atoms was considered. The average bond lengths are 1.42086Å and by using density functional theory the electronic structure calculations are performed. Fig.1.1 and Fig.1.2 shows the structure of CNT with one Lithium atom in both cases. All the models are in relaxed state and geometry optimization was applied. The deformation after geometry optimization is negligibly small.

Now we examined structures with multiple attachments of Lithium atoms inside and outside of the CNT. The structures with multiple Lithium atoms are shown in Fig. In both the cases lithium atoms are placed at an average distance of 2.50Å all the Li atoms are positioned symmetrically. Geometry optimization has been performed at every stage. From Fig.1.2 we can observe that before optimization atoms are in relaxed position and after that most of the Li atoms which are on the outside of the CNT was attaching with the nearby carbon atoms. But it is not happened when we inserted Li atoms inside CNT shown in Fig.1.1. The binding energies of multiple Li atoms with inside and outside is calculated and shown in Table 1.1

The electronic band structure of pristine (10, 0) CNT is 0.689eV, which shows that the carbon nanotube is a semiconductor and shown in Fig.1.3. It is compared with Li inserted CNT The differences can be observed in the band structures and density of states i.e. the semiconducting nature has been turned to metallic nature.

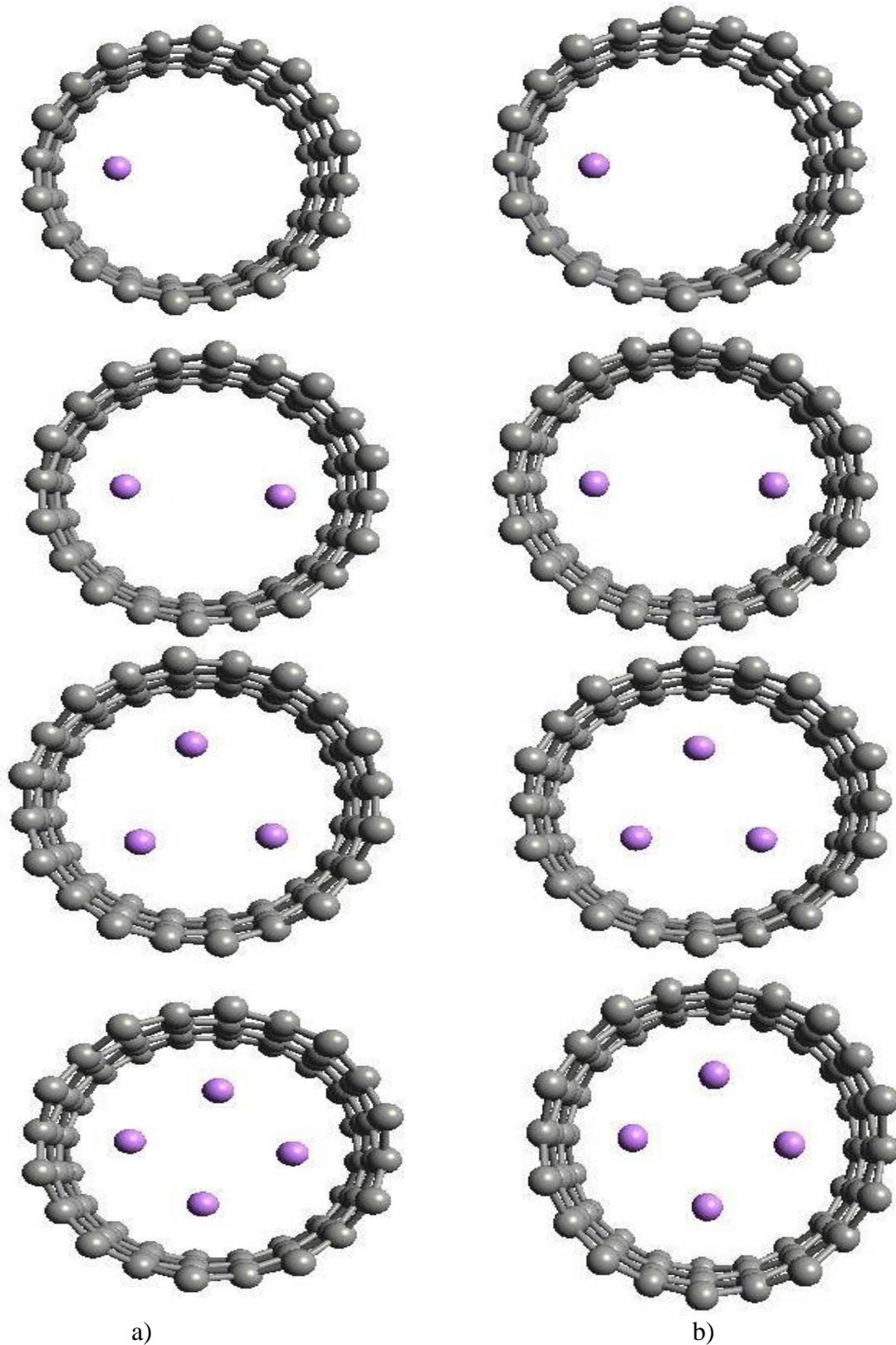


Figure 1.1: (10, 0) CNT inside Li atoms, Panel a, b shows structures before and after optimization respectively

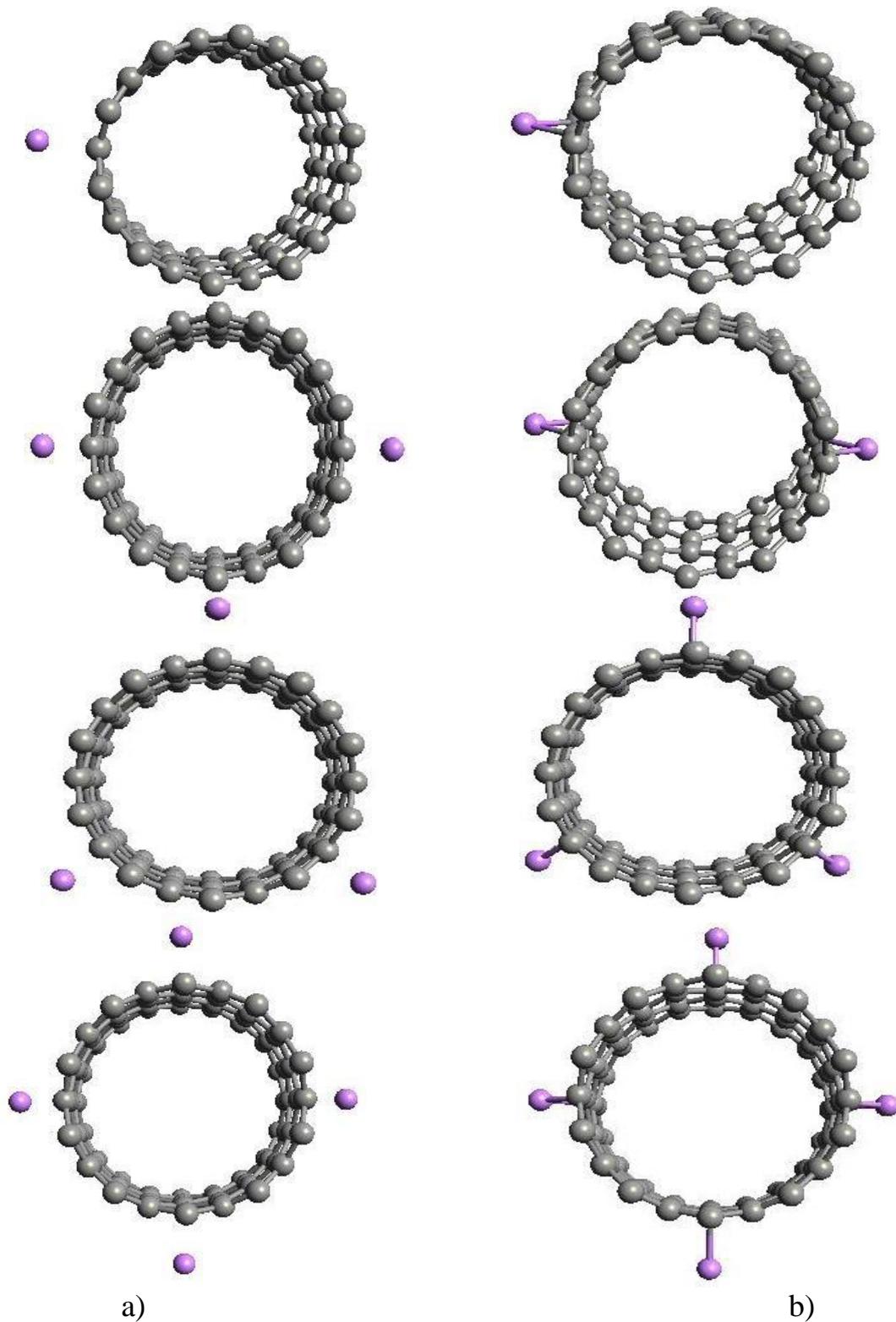


Figure 1.2: (10, 0) CNT outside Li atoms, Panel a, b shows structures before and after optimization respectively

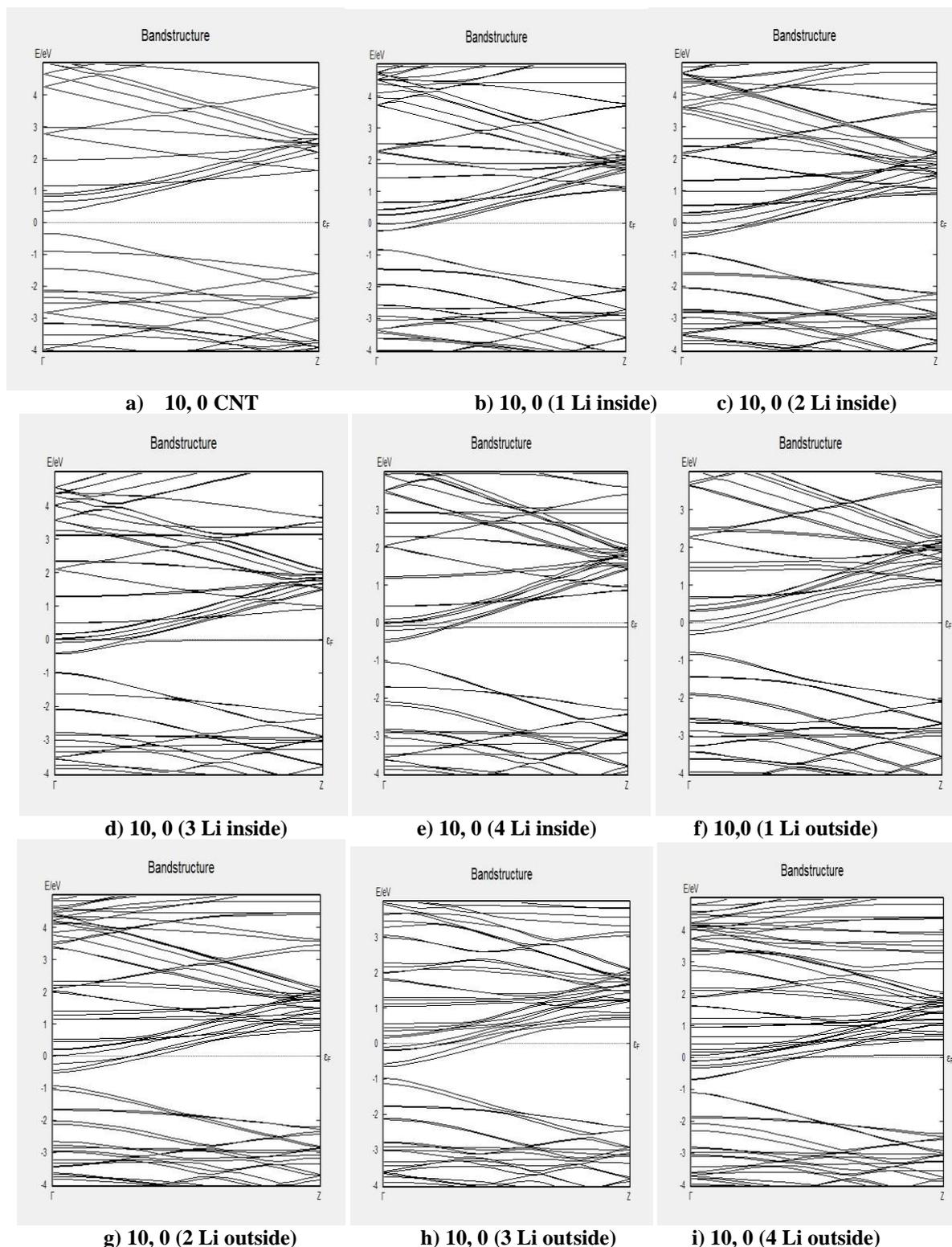
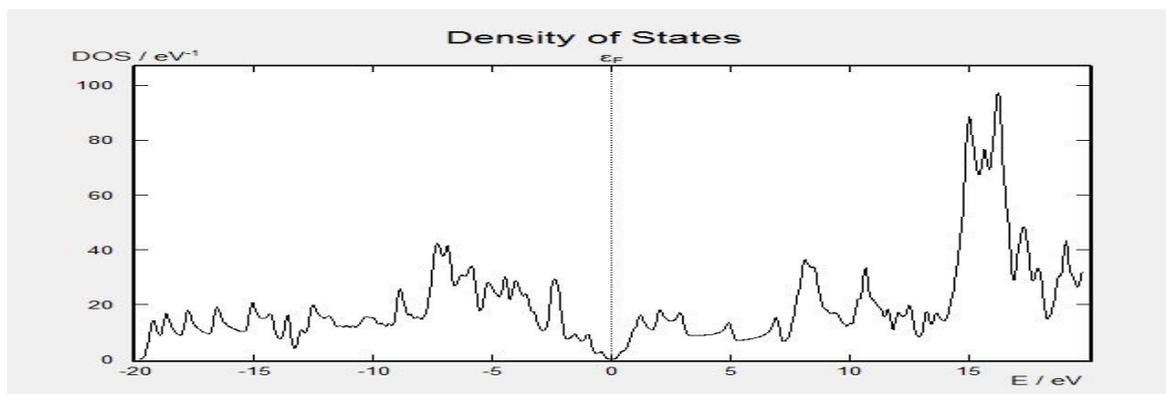
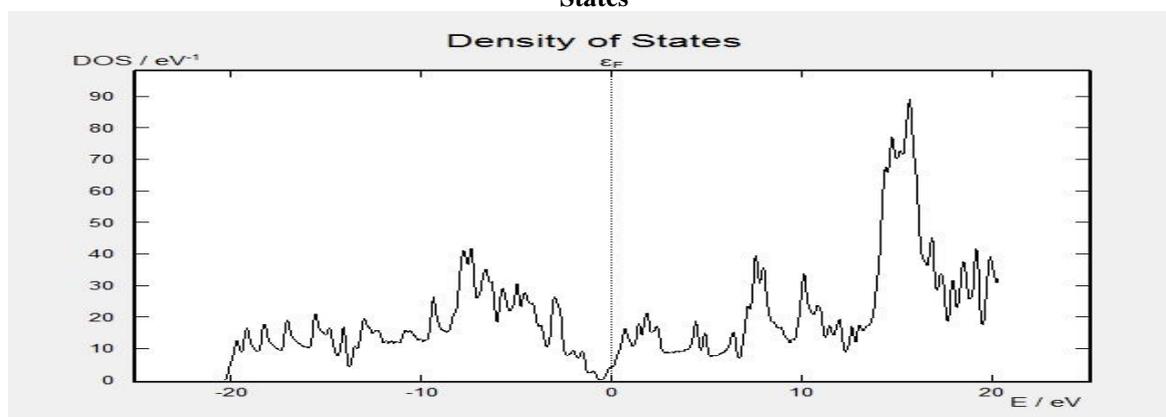


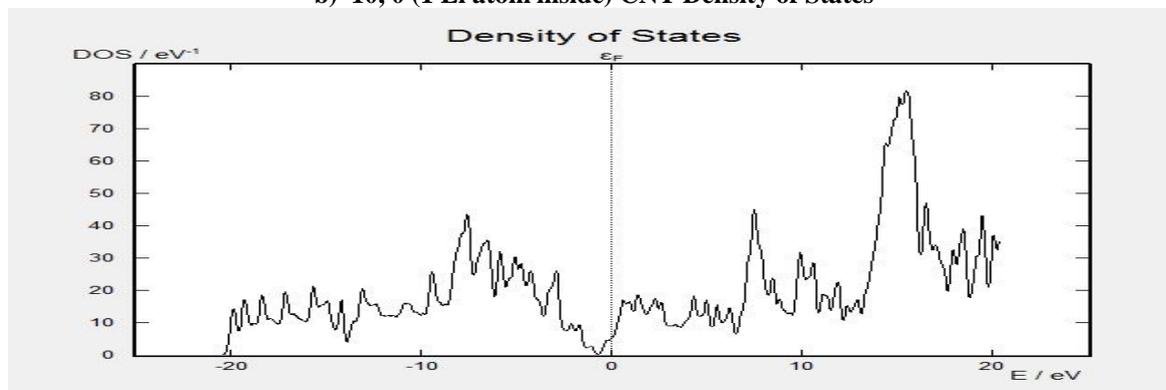
Figure 1.3: Band structure a) for (10, 0) CNT. Panel's b) to e): for (10, 0) with lithium atoms inside the CNT and Panel's f) to i): for (10, 0) with lithium atoms outside the CNT



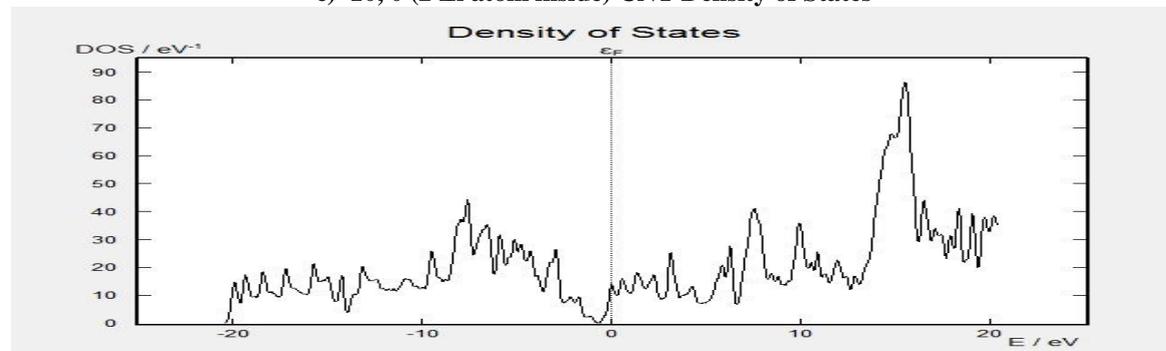
a) 10, 0 CNT Density of States



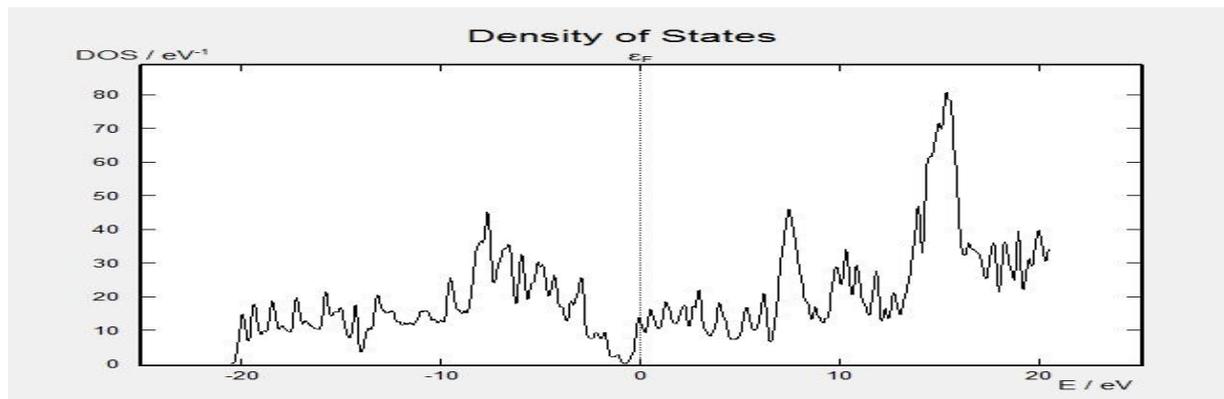
b) 10, 0 (1 Li atom inside) CNT Density of States



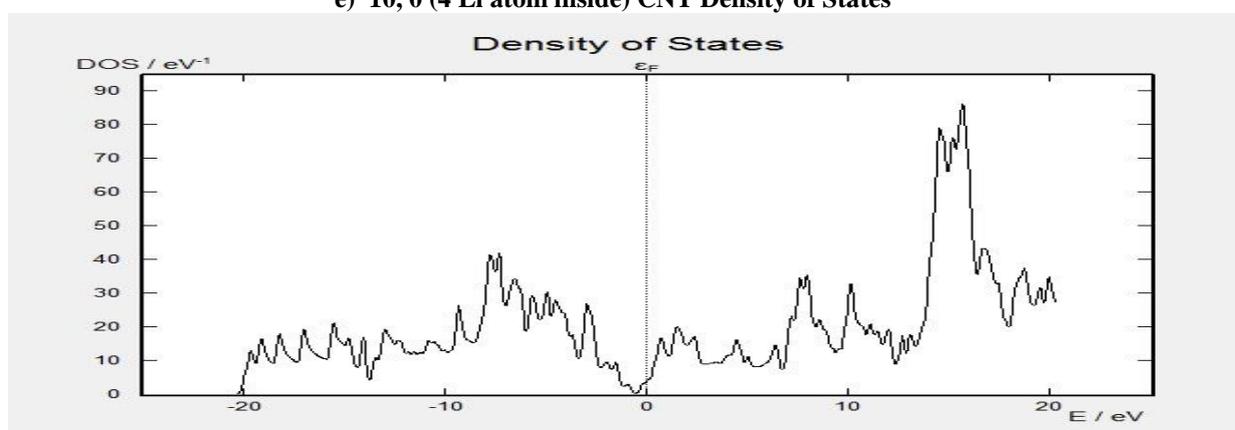
c) 10, 0 (2 Li atom inside) CNT Density of States



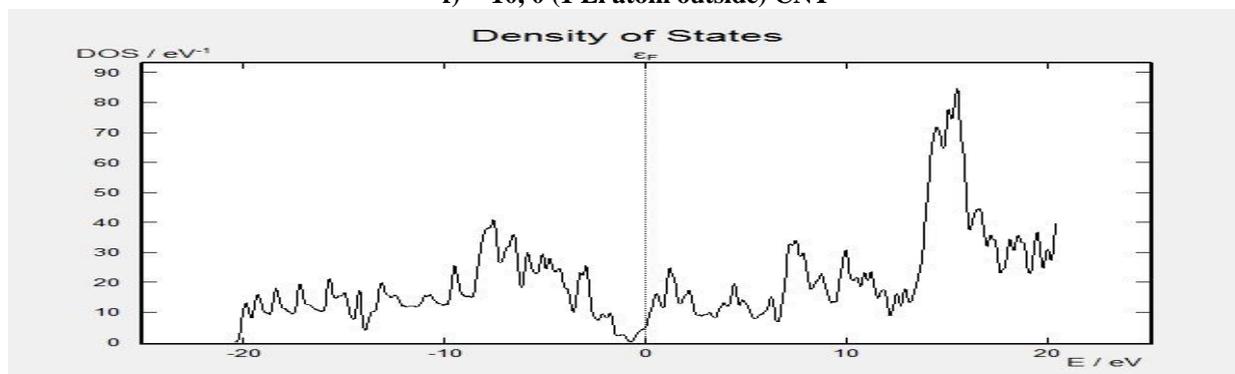
d) 10, 0 (3 Li atom inside) CNT Density of States



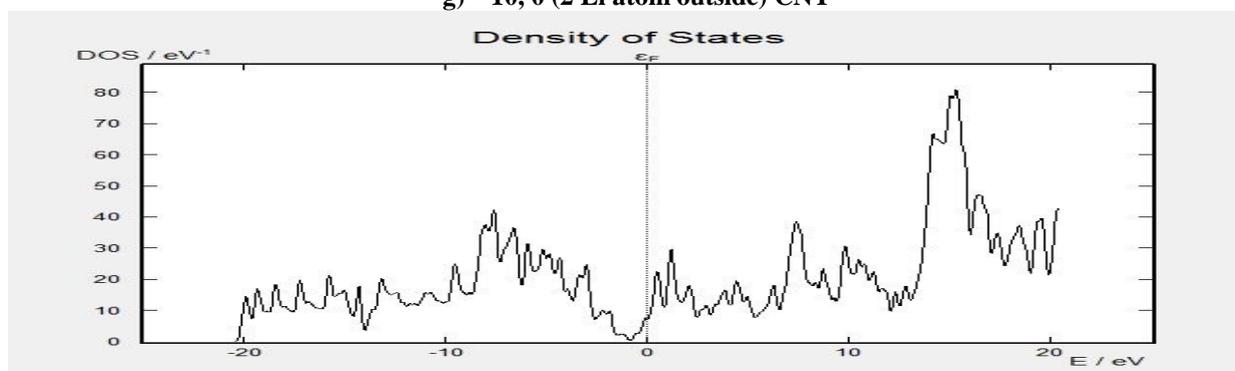
e) 10, 0 (4 Li atom inside) CNT Density of States



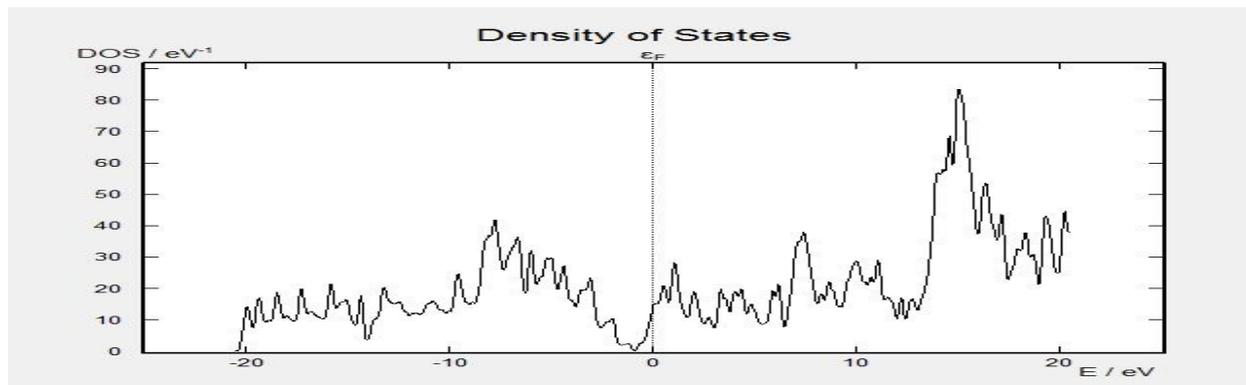
f) 10, 0 (1 Li atom outside) CNT



g) 10, 0 (2 Li atom outside) CNT



h) 10, 0 (3 Li atom outside) CNT



i) 10, 0 (4 Li atom outside) CNT

Figure 1.4: Density of states, a) for (10, 0) CNT. Panel's b) to e): for (10, 0) with lithium atoms inside the CNT and Panel's f) to i): for (10, 0) with lithium atoms outside the CNT.

Binding energies			
Inside		Outside	
10, 0 @ 1 Li	2.95	10, 0 @ 1 Li	2.05
10, 0 @ 2 Li	4.16	10, 0 @ 2 Li	4.33
10, 0 @ 3 Li	6.12	10, 0 @ 3 Li	7.02
10, 0 @ 4 Li	8.02	10, 0 @ 4Li	9.98

Table 1.1: Binding energies for (10, 0) CNT with Lithium atoms in both inside and outside

Therefore, when the lithium atoms placed inside of the (10, 0) CNT the binding energy is in the range of 2.95eV to 8.02eV whereas for the outside, it is in the range of 2.05eV to 9.98eV.

#### IV. CONCLUSION

In this study, we have investigated the adsorption of lithium atoms on both inside and outside of (10, 0) zigzag CNT. The lithium storage in outside of the CNT is better compared with inside, where curvature effect plays important role in inside of the CNT. Therefore, the outside storage is favorable than inside. The charge is transferred from Li atoms to CNT. The amount of charge transfer is higher for the outside attachment compared with the inside.

#### V. ACKNOWLEDGEMENTS

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