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A density functional Study of Interaction of Zn Atom on Single Walled Carbon Nanotube (8,0)

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ABSTRACT

First principal of density function theory was implemented to investigate interaction of Zinc (Zn) atom on pristine Single Walled Carbon Nanotube (SWCNT) (8, 0). To predict interaction we tested four different sites of adsorption and found electronic properties such as Band Structure (BS), Density of State (DOS), Energy Gap (EG), Binding Energy (EG), Charge transfer (Q_t) and geometrical properties such as change Bond length, Bond angle, Binding distance. The binding energy, energy gap and charge transfer shows that Zn atom is physisorbed on SWCNT. The electronic and geometrical properties of pristine SWCNT are minutely changed.

Keywords: Carbon Nanotube, DFT, SWCNT, Zinc.

INTRODUCTION

Carbon nanotubes have exceptional physical and chemical properties because of these chemists and physicists are trying to understand better through research[1,3]. Because of the bonding characteristics of carbon atoms, the physical appearance of carbon nanotubes can often resemble rolled up. Each carbon atom in a Carbon nanotube is connected via strong chemical bond to three neighboring atoms. Depending on the chiral indices, CNTs exhibit both metallic and semiconducting properties. CNTs can exhibit the strongest basal plane elastic modulus and hence are expected to be an ultimate high strength fiber. The elastic modulus of SWNTs is much higher than steel that makes them highly resistant. Although pressing on the tip of nanotube will cause it to bend, the nanotube returns to its original state as soon as the force is removed. This property makes CNTs extremely useful as probe tips for high resolution scanning probe microscopy.[4-8]

Tomorrow's world will be shaped by nanotube applications, just as silicon-based technologies which dominate society today. Space elevators tethered by the strongest of cables; hydrogen-powered vehicles; artificial muscles: these are just a few of the technol. marvels that may be made possible by the emerging science of carbon nanotubes. By optimization physical and chemical properties it becomes easier to predict their behavior which would ultimately make them more useful for possible nanosensors. These nanosensors could behave like semiconducting materials in microelectronic circuits, or detect small changes in electric current, or register chemical reactivity, or changes in air pressure or temperature.[9-13]

In this paper we will find whether Zn is suitable with carbon nanotube. As per our study no one has studied the zinc atom with CNT (8,0) and found its Isosurface , HOMO,LUMO. We will discuss in this paper.

COMPUTATIONAL METHOD:

We have chosen (8, 0) SWCNT and Au atom model using material studio by Accelrys which is a molecular dynamics simulation software. The geometrical and electronic properties of the system were derived using quantum mechanics program Dmol3 code (Accelrys) .we used GGA and PBE method for optimization.

For Supercell geometries, spin unrestricted calculations were carried out with a double numeric polarized (DNP) basis set available and orbital cut-off set to 4.4 Å. Scalar relativistic effects were included via a pseudo potential for all-electron calculations. 1 × 1 × 2 k-points were used for the Brillioun zone. All the calculations were performed using boundary conditions with 64 atoms within the Supercell. The tetragonal unit cell of 20 × 20 × 8.4 Å dimensions and sufficient separation between tubes is used to avoid interaction between the atoms. The chosen cut off value leads to atomic energies with an accuracy of 0.1eV/atom, allowing calculations without sufficient loss of accuracy. The calculations were performed to find the structural and electronic properties of optimized structures. Milliken population analysis was carried out to predict the charge transfer and spin between Zn-Atom and nanotubes.

COMPUTATION DETAILS:

We have selected (8, 0) zigzag CNT of diameter 6.26 Å and the length of tube is 8.52Å as a model to study the adsorption of Zinc atom. We have examined different site for adsorption of Zn atom as shown in figure (1). 1) Carbon Atom (Site A), 2) Carbon-Carbon Axial Bond (site B), 3) Carbon-Carbon Chiral bond (site C) and 4) Hexagon (site D). In all calculations, the carbon nanotubes along with Zn atom were first optimized to occupy their minimize energy state. For each site Zn has kept at a finite distance of 3.0 Å to optimize the system to get stable structure. The binding energy (E_b) of adsorption of Zn atom on nanotube for all ground state structures were calculated by

$E_b = - [E_T (\text{adsorbent} + \text{adsorbate}) - E_T(\text{adsorbent}) - E_T(\text{adsorbate})]$.

Where E_T (adsorbent + adsorbate) is the total energy of atom and CNT system, E_T (adsorbent) is total energy of CNT and E_T (adsorbate) is the total energy of atom. To verify the computational accuracy of the structure we have calculated the binding energy of CNTs, density of state, band gap Charge Density, Milliken Charge.

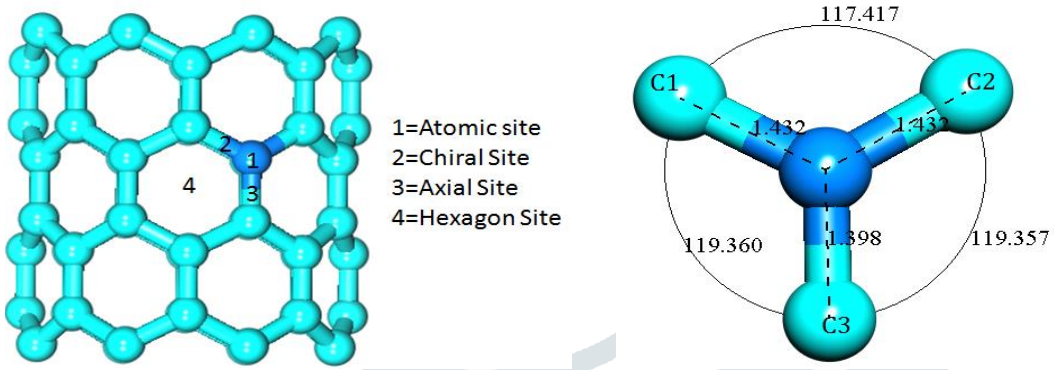


Figure1: (a) Structural model of CNT (8, 0) (b) structural parameter at target atom

Result and discussion:

Zinc is a bluish-white, lustrous, diamagnetic metal, though most common commercial grades of the metal have a dull finish. Zinc is a chemical element with symbol Zn and atomic number 30. It is the first element in group 12 of the periodic table. It is somewhat less dense than iron and has a hexagonal crystal structure, with a distorted form of hexagonal close packing, in which each atom has six nearest neighbors (at 265.9 pm) in its own plane and six others at a greater distance of 290.6 pm. Zinc is a fair conductor of electricity.

1. Structural Properties:

The (8,0) SWCNTs presented in Figure 1. has a carbon atom arrangement with an average C-C bond length of 1.432 Å at chiral bond length and 1.398Å for axial bond length. One carbon atom was chosen for exo-interaction of atom. Geometry optimization of the all four positions resulted in slight increase in bond length of chiral and axial positions of SWCNT. Figure 2 and 3 displays the after optimization carbon-carbon bond length and Zn-SWNT bond length, result is tabulated in table 1.

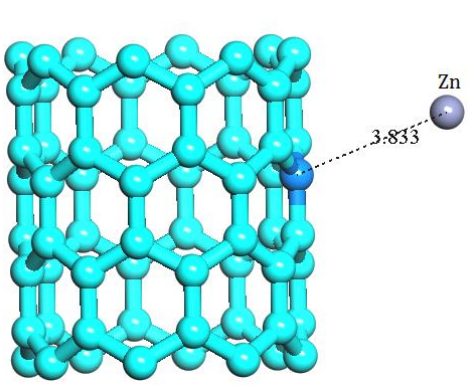
Site	Bond Length(Å)	Bond Angle(°)	Hybridization of CNT
Zn Atomic	3.833 Å	c1-c-c3=117.299, c1-c-c2=119.336, c3-c-c2=119.318	SP^2
Zn Atomic bond	3.831 Å	c1-c-c3=117.299, c1-c-c2=119.336, c3-c-c2=119.318	SP^2
Zn AXIAL	3.898 Å	c1-c-c3=117.449, c1-c-c2=119.361, c3-c-c2=119.358,Zn-C=20.664°	SP^2

Zn Axial bond	3.894 Å	c1-c-c3=117.449, c1-c-c2=119.361, c3-c-c2=119.358,Zn-C=20.686	SP^2
Zn Chiral	4.029Å_3.975 Å	c1-c-c3=117.337, c1-c-c2=119.323, c3-c-c2=119.321,Zn-C=20.6	SP^2
Zn Chiral Bond	3.879Å_4.109Å	c1-c-c3=117.337, c1-c-c2=323, c3-c-c2=119.321,Zn-C=20.399	SP^2
Zn Hexagon	4.065Å_4.060Å	c1-c-c3=117.454, c1-c-c2=119.349, c3-c-c2=119.365, a1=19.801,c1=20.615,c2=20.648,c-c=35.066	SP^2
Zn Hexagon Bond	4.065Å_4.061Å	c1-c-c3=117.454, c1-c-c2=119.349, c3-c-c2=119.365 a1=19.801,c1=20.615,c2=20.648,c-c=35.067	SP^2

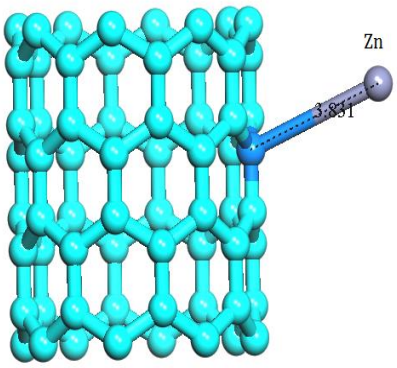
Table 1: Bond Length and Bond angle for Zn-CNT geometry optimization

Before optimization, in the prepared model the distance of adsorption of Zn adatom is about 3.0 Å from carbon atom or carbon-carbon bond. After performing Geometry optimization Zn adatom get Physisorbed to carbon atom of nanotube by bond length from 3.83 Å to 4.109 Å at all four positions selected for interaction. From bond length we have observe that atom all four positions Zn atom get physisorbed. We can see the change in bond length at atomic, axial, chiral and Hexagon position of CNT during the interaction of Zinc (Zn) as shown in table 1.

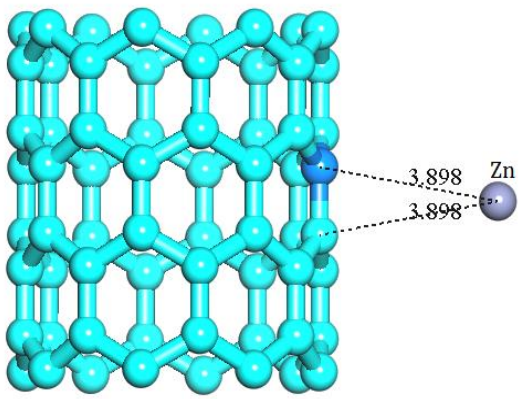
The bond angles between C - C - C bonds were ranging from117.2º to 119.4º which is less than 120º indicates trigonal structure of bonding and prefers SP^2 hybridization as shown in Table 1.



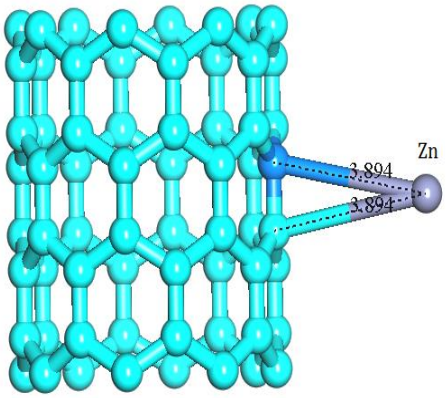
1)Atomic



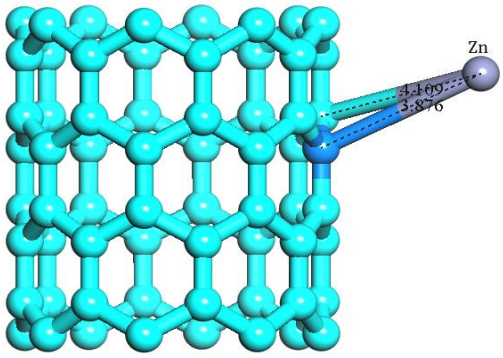
Atomic Bond



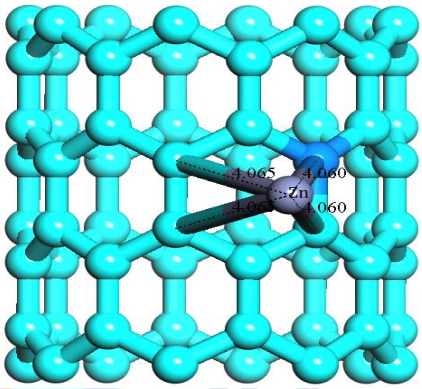
2) Axial position



Axial Bond



3. Chiral Bond



4. Hexagon position

Figure 2: Stable Geometry of Zn-SWCNT at (1)Atomic (2) axial (c) Chiral (d) Hexagon

2.Electronic Properties

- Binding Energy(B.E)

The Binding energy of pure (8, 0) SWCNT, molecule and Zn-SWCNT were calculated. The Binding energy determines the stability of the system and the higher binding energy shows lower the stability of the system. Table 2. Shows the summery of calculated binding energy of the studied system, where positive value of binding energy indicates a gain of energy and negative value shows the loss of energy.

Table 2. Binding Energy of Zn-SWCNT

Structure type	B.E in eV
Zn-SWCNT(Atomic without bond)	-0.0463
Zn-SWCNT(Atomic bond)	-0.0436
Zn -SWCNT(Axial without bond)	-0.03
Zn -SWCNT(Axial bond)	-0.03
Zn -SWCNT(chiral without bond)	-0.0409
Zn -SWCNT(chiral bond)	-0.0436
Zn -SWCNT(Hexagon without bond)	-0.0436
Zn -SWCNT(Hexagon bond)	-0.0436

From Above table-2 we can conclude that Zn interaction with SWCNT in all four positions with and without bond is less stable. So no bond formation taking place.

- Charge Transfer:

  Mulliken charge analysis was used to calculate the charge transfer between the CNTs the metal interaction calculations were done as shown in table. Metal atoms gains electron from the surrounding carbon atoms, but very less amounts of electrons is gain when Zn atom interacted and no spin is present with CNT as shown in Table 3.

Table 3: Charge Transfer

Structure type	Mulliken Charge	Spin
Zn-SWCNT(Atomic without bond)	0.011	0
Zn-SWCNT(Atomic bond)	0.011	0
Zn -SWCNT(Axial without bond)	0.007	0
Zn -SWCNT(Axial bond)	0.007	0
Zn -SWCNT(chiral without bond)	0.01	0
Zn -SWCNT(chiral bond)	0.012	0
Zn -SWCNT(Hexagon without bond)	0.011	0
Zn -SWCNT(Hexagon bond)	0.011	0

Figure shows the iso-surface of charge density. It shows no formation of bond between Zn atom and carbon atoms.

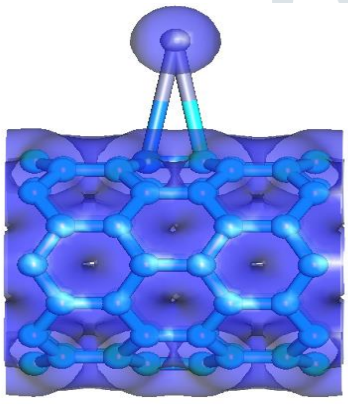


Figure: Isosurface of Zn-SWCNT at axial bond position.

2. Band Gap: Band gap calculations were performed for pure SWCNT (8, 0) & Zn-SWCNT interaction. This interaction of Zn atom with SWCNT shows almost no change in the band gap

Table 4: Band gap of Zn-CNT at different positions

Structure type	Band gap(eV)
Pure SWCNT(8,0)	0.70
Zn-SWCNT(Atomic without bond)	0.689
Zn-SWCNT(Atomic bond)	0.689
Zn -SWCNT(Axial without bond)	0.69

Zn -SWCNT(Axial bond)	0.69
Zn -SWCNT(chiral without bond)	0.689
Zn -SWCNT(chiral bond)	0.686
Zn -SWCNT(Hexagon without bond)	0.69
Zn -SWCNT(Hexagon bond)	0.69

The Band Structure (BS) and Density of State (DOS) of pure SWCNT is Shown in figure 4(a). The energy band gap found from BS and DOS for pure CNT is 0.701, which is competent to theoretically and experimentally reported result. Figure 4(b) shows BS and DOS for interaction of Zn atom with CNT at four different sites. BS and DOS for atomic site – 1, axial bond site – 3 and chiral bond site – 2, Hexagon bond site -4, In all four positions we got same bang gap as shown in table 4. So from Band structure and DOS also it shows that Zn does not interact with carbon in exo-doped.

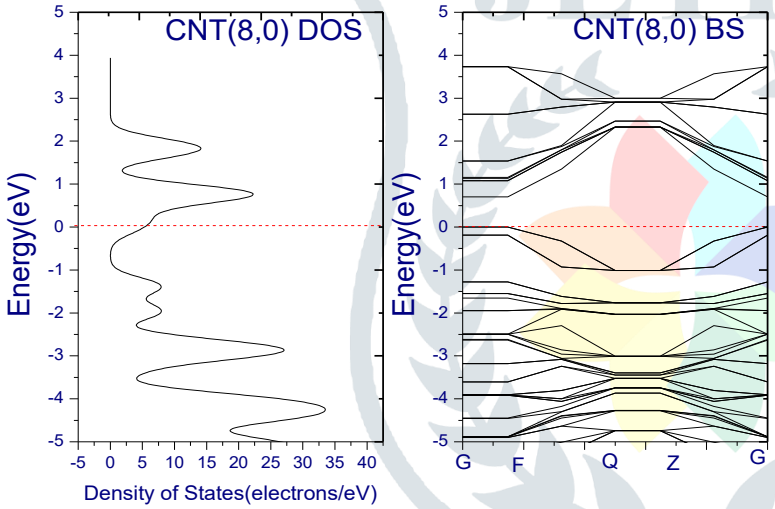


Fig 4(a) :DOS and BS of Pure CNT(8,0)

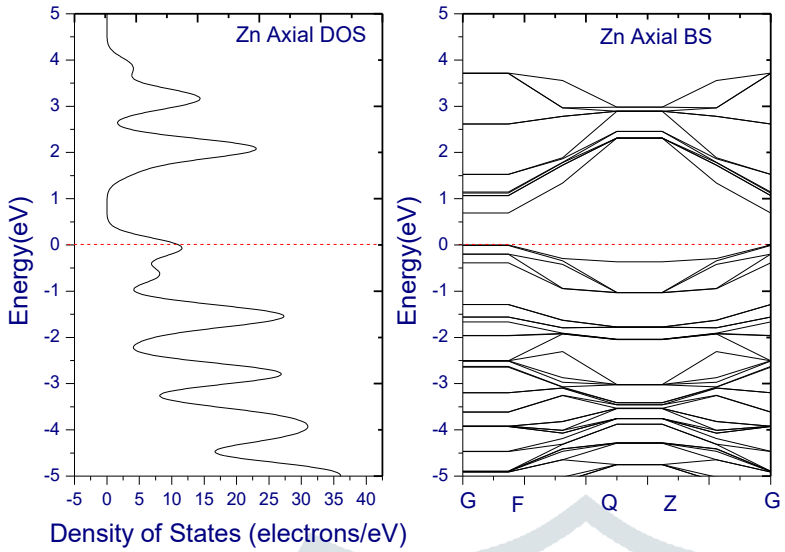


Fig4(b): DOS and BS in All four(Atomic,Axial,Chiral,Hexagon) positions of Zn-SWCNT

CONCLUSION:

The density functional theory based on linear combination of atomic orbital is used to study the adsorption of Zinc atom on CNT at various four sites. In all four adsorption site Zn atom is Physisorbed onto CNT by forming no bonds with carbon atom. Zn atom does not create any extra states near the Fermi energy level we have shown in DOS and BS. We also found that there is negligible charge transfer from Zn to CNT which does not change the properties of CNT which is semiconductor. The charge density and molecular orbital clearly shows no formation of bond between zinc and carbon atoms. Zn exo interaction does not change the properties of CNT so we conclude Zn cannot be used for any electronic devices.

Acknowledgements

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