

## Dielectric constant and polarizability in C64 carbon nanotube; A first-principles study

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### ABSTRACT

First-principles calculations have been carried out on a Carbon Nanotube C64. The Electronic density of states reveals that the material shows metallic nature. The value of dielectric constant in Carbon Nanotube C64 comes out to be 20.7, 16.5 and 14.6 along X, Y and Z axes respectively and its average value comes out to be 17.3. Polarizability of Carbon Nanotube C64 has been estimated and it comes out to be  $87.3 \text{ (\AA)}^3$ ,  $84.3 \text{ (\AA)}^3$  and  $82.5 \text{ (\AA)}^3$  along X, Y and Z axes respectively.

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### KEYWORDS

Carbon nanotube;  
EDOS;  
First-principles calculations;  
Dielectric constant;  
Polarizability.

### INTRODUCTION

Ever since their discovery in 1991<sup>[1]</sup>, Carbon nanotubes have been the subject of intense research. Single Walled Carbon Nanotubes (SWCNTs) have gained particular attention because of the wide range of potential applications from structural materials with extraordinary mechanical properties<sup>[2]</sup> to the preparation of nanoelectronic components<sup>[3]</sup>. SWCNTs can help in protecting DNA molecules from damage by oxidation<sup>[4]</sup>. It has been found that SWCNTs can also act as probe tips for scanning probe microscopy<sup>[5]</sup>. Carbon nanotubes and their polymer nanocomposites are found to be suitable scaffold materials for bone tissue engineering and bone formation<sup>[6]</sup>.

It has been found that any little modification in the structure and composition of a material will bring in sufficient changes in the properties of the mate-

rial<sup>[7,8]</sup>. Thus it is important to study the structure of the materials and look at the parameters which can be altered to get a better material for technological applications. First-principles calculation based on Density Functional Theory<sup>[9]</sup> has been proved to be an effective tool in the study of structural, electronic and dielectric properties of organic materials<sup>[10,11]</sup>. Carbon nanotubes have attracted the scientific community in various aspects. With this in view, structure of a Carbon Nanotube C64 has been simulated using First-principles calculations based on Density Functional Theory and computation of Electronic density of states, Dielectric constant and Polarizability have been done and the results have been reported in the present paper.

### Computational details

Several codes are available for the theoretical structure simulation<sup>[12]</sup>. The density functional theory approach has emerged as a well established com-

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putational method. It has been widely employed to arrive at the conformations of a large number of molecular systems. The practical applicability and sophistication of DFT is strongly sensitive to the good choice of exchange–correlation function along with the appropriate basis set.

Quantum espresso is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modelling. It is based on density-functional theory, plane waves, and pseudopotentials. Author has used plane wave self consistent field (PWSCF)<sup>[13]</sup> implementation of density functional theory (DFT), with a Local density approximation (LDA)<sup>[14]</sup> to exchange correlation energy of electrons and ultrasoft pseudopotentials<sup>[15]</sup>, to represent interaction between ionic cores and valence electrons. Kohn-Sham wave functions were represented with a plane wave basis with an energy cutoff of 30 Ry and charge density cutoff of 180 Ry. Integration over Brillouin zone was sampled with a Monkhorst-Pack scheme<sup>[16]</sup> with appropriate k point mesh and occupation numbers were smeared using Methfessel-Paxton scheme<sup>[17]</sup> with broadening of 0.03 Ry. The structure was relaxed to minimize energy.

## RESULTS AND DISCUSSION

In the present study, the Tetragonal unit cell of Carbon Nanotube C64 was first simulated (with  $m=8$

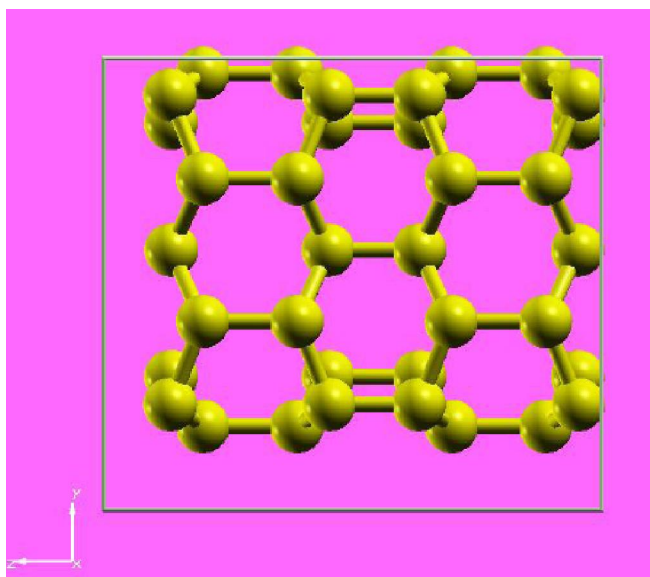


Figure 1 : Structure of unit cell of carbon nanotube C64 as viewed along X-axis

and  $n=0$ ) using “Avogadro”<sup>[18]</sup>. Later, atomic positions of the simulated structure have been used in the plane wave self consistent field calculations.

The structure was relaxed and the optimized values of the unit cell parameters thus arrived at through minimization of energy are;  $a=b=7.25\text{\AA}$  and  $c=8.02\text{\AA}$ , “scf” calculation was done using the final atomic positions obtained after relaxing the struc-

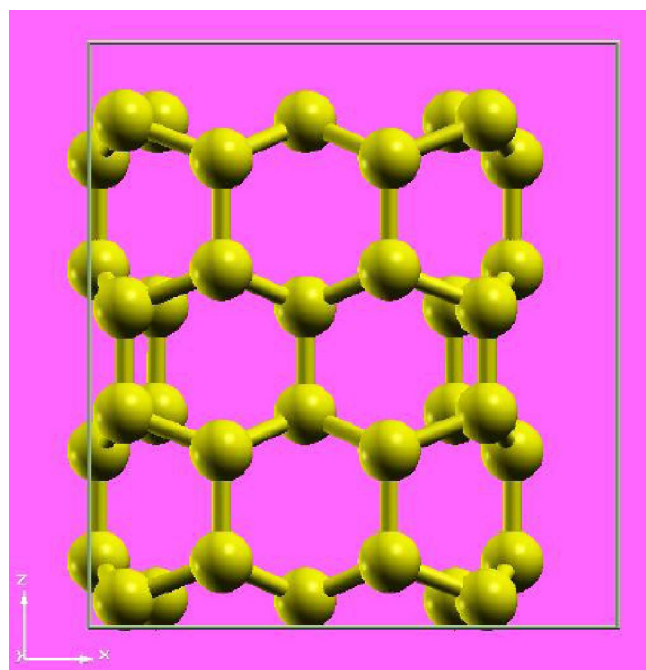


Figure 2 : Structure of unit cell of carbon nanotube C64 as viewed along Y-axis

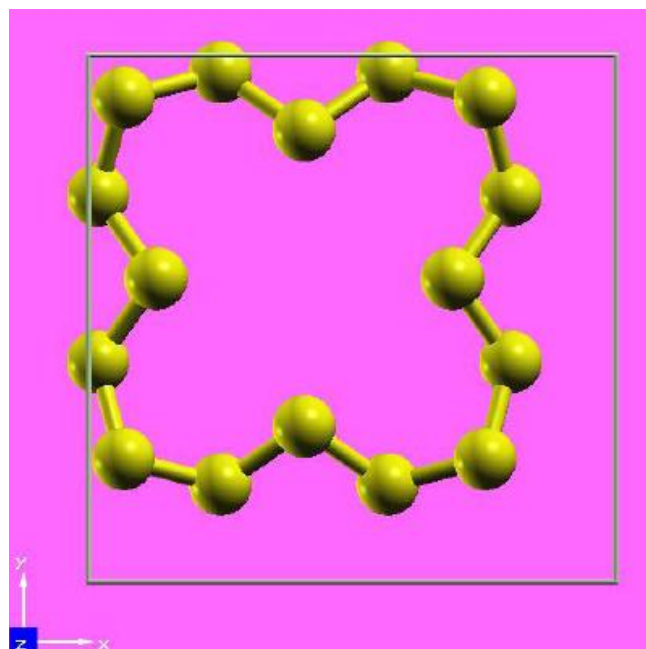


Figure 3 : Structure of unit cell of carbon nanotube C64 as viewed along Z-axis.

ture using the program 'pw.x' of Quantum espresso.

Completely relaxed structure of the unit cell was visualized using the program "XcrysDen"<sup>[19]</sup> and the structure of unit cell of Carbon Nanotube C50H10 as seen along X, Y and Z axes are shown in Figures

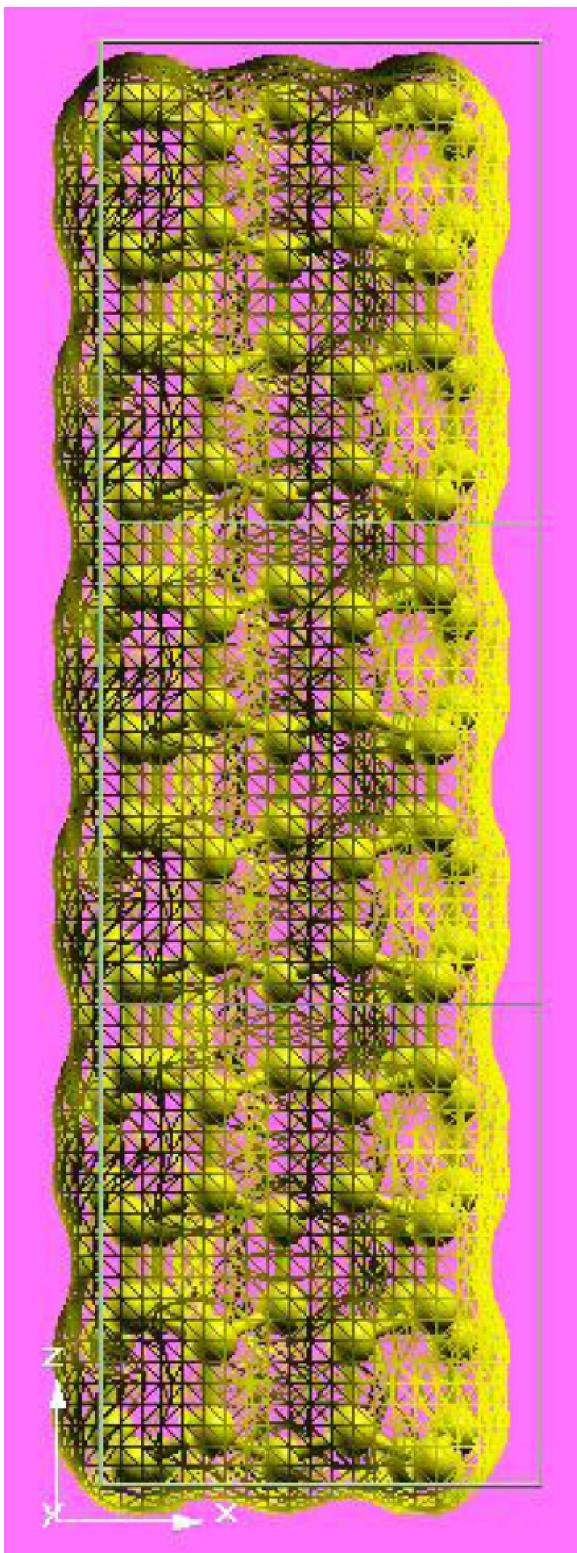


Figure 4 : Molecular surface of carbon nanotube C64

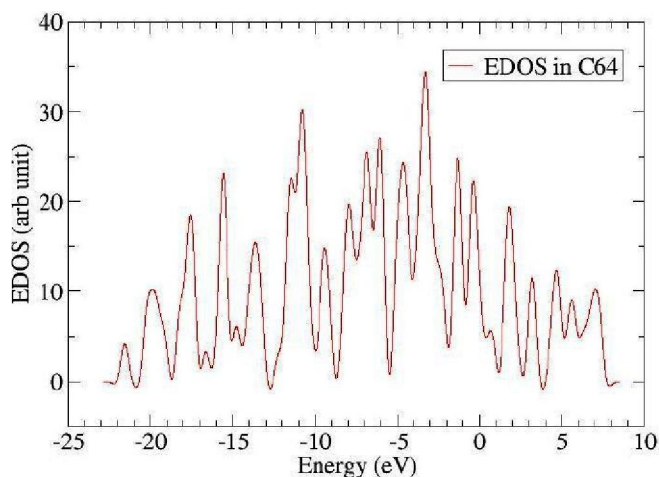


Figure 5 : Electron density of states in carbon nanotube C64

1, 2 and 3 respectively. The molecular surface of the Carbon Nanotube C64 is shown in Figure 4.

### EDOS Calculation

Electron Density of States (EDOS) has been computed in Carbon Nanotube C64 using Electronic structure calculation code of Quantum espresso. EDOS in Carbon Nanotube C64 has been shown in Figure 5. As it can be seen from the Figure 5, the material shows metallic nature without showing any band gap.

### Dielectric constant and polarizability

Dielectric constant has been computed in case of Carbon Nanotube C64. The value of dielectric constant in Carbon Nanotube C64 comes out to be 20.7, 16.5 and 14.6 along X, Y and Z axes respectively and its average value comes out to be 17.3. Polarizability of Carbon Nanotube C64 has also been estimated and it comes out to be  $87.3 \text{ (\AA)}^3$ ,  $84.3 \text{ (\AA)}^3$  and  $82.5 \text{ (\AA)}^3$  along X, Y and Z axes respectively.

### CONCLUSIONS

The simulated and optimized structure of Carbon Nanotube C64 shows that the tube extends along Z direction. The EDOS calculation shows that the material shows metallic nature without showing any band gap. The average value of dielectric constant comes out to be 17.3. Polarizability comes out to be  $87.3 \text{ (\AA)}^3$ ,  $84.3 \text{ (\AA)}^3$  and  $82.5 \text{ (\AA)}^3$  along X, Y and Z axis respectively.

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