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First-Principles Study of Dielectric Constant and Polarizability in Two Carbon Nanotubes

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Abstract **- First-principles calculations have been carried out on two Carbon Nanotubes having 54 and 72 carbon atoms. The Electronic density of state reveals that the materials show metallic nature. Dielectric constant has been computed in case of Carbon Nanotubes C54 and C72. The value of dielectric constant in Carbon Nanotube C54 comes out to be 7.06, 6.28 and 14.53 along X, Y and Z axes respectively and its average value comes out to be 9.29. Value of dielectric constant in Carbon Nanotube C72 comes out to be 167, 168 and 737 along X, Y and Z axes respectively and its average value comes out to be 357. Polarizability of Carbon Nanotube C54 has been estimated and it comes out to be 116(Å)^3, 111(Å)^3 and 142(Å)^3 along X, Y and Z axis respectively. Polarizability in case of Carbon Nanotube C72 comes out to be 171(Å)^3, 171(Å)^3 and 173(Å)^3 along X, Y and Z axes respectively.**

Keywords**: Carbon Nanotube, EDOS, First-principles calculations, Dielectric constant, Polarizability**

I. INTRODUCTION

Since their discovery in 1991 [1], 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 [2] to the preparation of nanoelectronic components [3]. SWCNTs can help in protecting DNA molecules from damage by oxidation [4]. It has been found that SWCNTs can also act as probe tips for scanning probe microscopy [5]. Carbon nanotubes and their polymer nanocomposites are found to be suitable scaffold materials for bone tissue engineering and bone formation [6 - 9].

Several methods of synthesis of Carbon Nanotues have been proposed and several structure related properties have been investigated [10 – 14]. There are several other proposed applications of nanotubes which include high-sensitivity microbalances [15], gas detectors [16,17], and hydrogen energy storage devices [18]. Their use in field-emission mode for displays [19,20] and as electrodes for organic light-emitting diodes [21] has substantial future technological potential.

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 material [22, 23]. 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 [24] has been proved to be an effective tool in the study of structural, electronic and dielectric properties of organic materials [25, 26]. Carbon nanotubes have attracted the scientific community in various aspects. With this in view, structure of a Carbon Nanotubes C54 and C72 have 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.

II. COMPUTATIONAL DETAILS

Several codes are available for the theoretical structure simulation [27]. The density functional theory approach has emerged as a well-established computational 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) [28] implementation of density functional theory (DFT), with a Local density approximation (LDA) [29] to exchange correlation energy of electrons and ultrasoft pseudopotentials [30], 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 [31] with appropriate k point mesh and occupation numbers were smeared using Methfessel-Paxton scheme [32] with broadening of 0.03 Ry. The structure was relaxed to minimize energy.

III. RESULTS AND DISCUSSION

In the present study, the Tetragonal unit cell with parameters a=b=7.49Å and c=12.98Å containing the Carbon Nanotubes with 54 and 72 carbon atoms were first simulated using

"Avogadro" [33]. Later, atomic positions of the simulated structure have been used in the plane wave self-consistent field calculations. "scf'" calculation was done using the final atomic positions obtained after relaxing the structure using the program 'pw.x' of Quantum espresso.

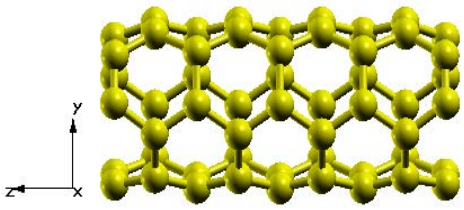

Fig.1 Structure of Carbon Nanotube (C54) as viewed along X-axis

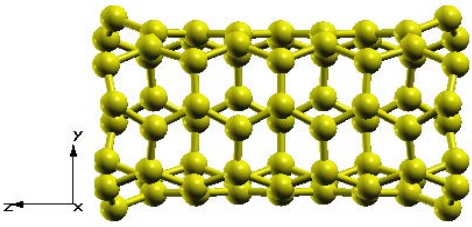

Fig.2 Structure of Carbon Nanotube (C72) as viewed along X-axis

Relaxed structure of the unit cell was visualized using the program "XcrysDen"[34] and the structure of unit cell of Carbon Nanotubes C54 and C72 as seen along X-axis are shown in Figures 1 and 2 respectively.

A. EDOS Calculation

Electron Density of States (EDOS) has been computed in Carbon Nanotubes C54 and C72 using Electronic structure calculation code of Quantum espresso. EDOS in Carbon Nanotubes C54 and C72 have been shown in Figures 3 and 4 respectively. As it can be seen from the figures 3 and 4, both the materials show metallic nature without showing any band gap.

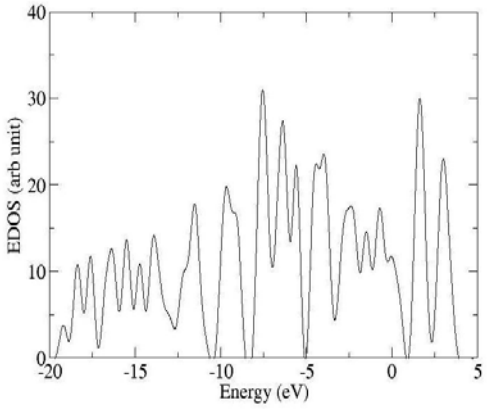

Fig. 3 Electron Density of States in Carbon Nanotube C54

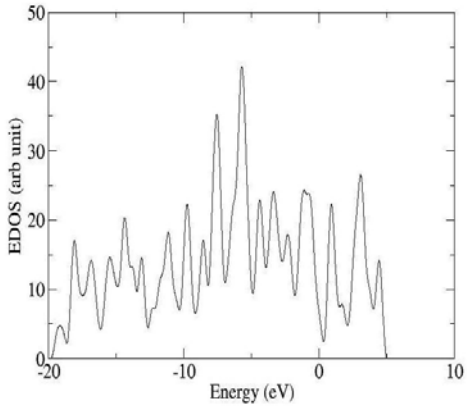

Fig. 4 Electron Density of States in Carbon Nanotube C72

B. Dielectric Constant and Polarizability

Dielectric constant has been computed in case of Carbon Nanotube C54 and Carbon Nanotube C72. The value of dielectric constant in Carbon Nanotube C54 is found to be 7.06, 6.28 and 14.53 along X, Y and Z axes respectively and its average value comes out to be 9.29. Value of dielectric constant in Carbon Nanotube C72 comes out to be 167, 168 and 737 along X, Y and Z axes respectively and its average value comes out to be 357. Polarizability of Carbon Nanotube C54 has also been estimated and it comes out to be 116(Å)^3, 111(Å)^3 and 142(Å)^3 along X, Y and Z axes respectively. Polarizability in case of Carbon Nanotube C72 comes out to be 171(Å)^3, 171(Å)^3 and 173(Å)^3 along X, Y and Z axes respectively. Thus the values of dielectric constant and polarizability are found to increase with increase in number of carbon atoms.

IV. CONCLUSION

The simulated and optimized structure of Carbon Nanotubes C54 and C72 show that they extend along Z direction. The EDOS calculations show that both the materials show metallic nature without showing any band gap. The value of dielectric constant and polarizability is large in both cases. The values of dielectric constant and polarizability are found to increase with increase in number of carbon atoms.

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