DENSITY OF STATES OF SINGLE-WALLED CARBON NANOTUBES : A COMPUTATIONAL COMPARATIVE STUDY

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This paper reports the density of states (DOS) of chiral (4,1), armchair (4,4), and zigzag ((4,0) single-walled carbon nanotubes (SWCNTs) by using ab-initio Density Functional Theory (DFT). Our simulation results show the distinguishable features of three types of CNTs in terms of density of states (DOS), so that they can be fully exploited in nano-devices. The results are helpful for studying the working principles of the CNT-based electronic devices and designing new ones.

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Introduction

Among one-dimensional nanostructures carbon nanotubes (CNTs)[1,2] are the most explored one and have attracted tremendous interest from both fundamental science and technological perspectives. CNT is a rolled one atom thick layer called graphene, where the length of the tube is larger than the tube diameter.[3] These nanostructures are topologically simple and exhibit a rich variety of intriguing electronic properties such as metallic and semiconducting behaviour.[3,4] Furthermore, these structures are atomically precise, meaning that each carbon atom is still three-fold coordinated without any dangling bonds. CNTs show a wide range of applications in the area of electronic, optics, medical, mechanics, and in many other industrial areas.[5-11] Therefore, much attention has been given to the investigation of their electrical, vibrational and thermal properties of CNTs.[12-16]

The electronic transport properties of two-probe system of heterojunction formed by an (8, 0) CNT and an (8, 0) silicon carbide nanotube (siCNT) has been reported Liu et al.,[17] whereas Anders Blom et al.[18] investigated the InAs p-i-n junction and calculated the transport characteristics of the system using two different approaches. In this work, we calculated the density of states (DOS)of chiral, armchair and zigzag SWCNTs by using density function (DFT) calculation of atomistic toolkit (ATK) software.

Results and Discussions

The carbon–carbon bond lengths of the simulated (4,1), (4,4) and (4,0) carbon nanotube structures are taken as 1.423 Å whereas the lengths of the central regions of the simulated sections are taken as 3 periods. The geometries of the simulated structures are shown in Figure 1a-1c.

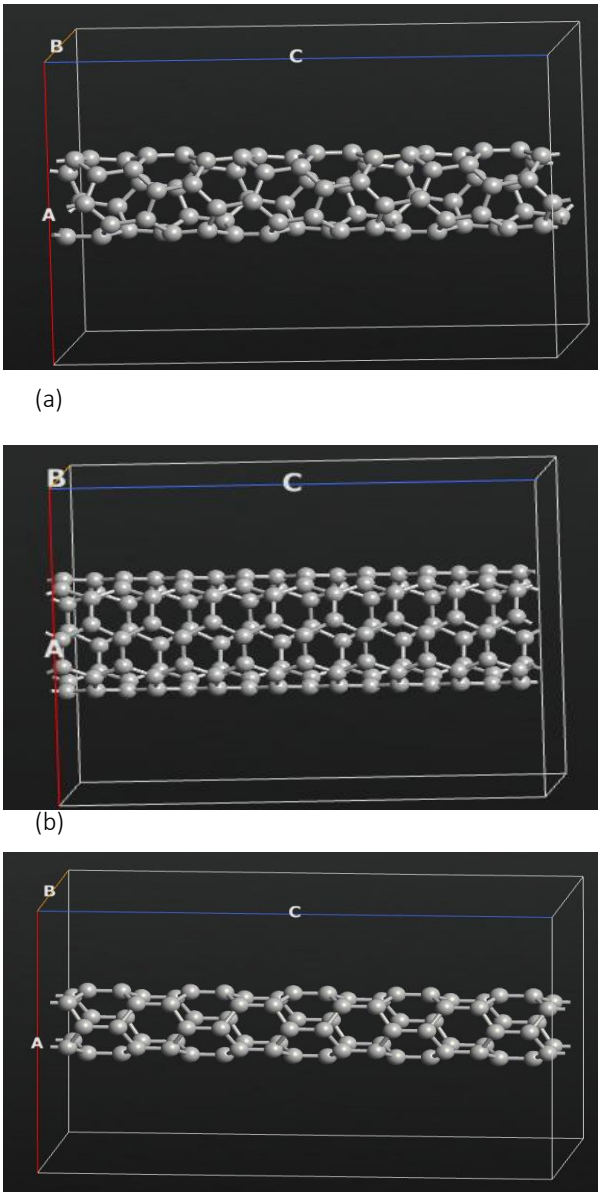
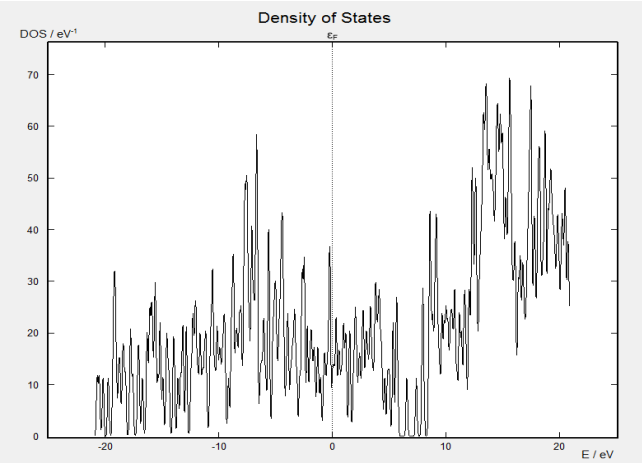
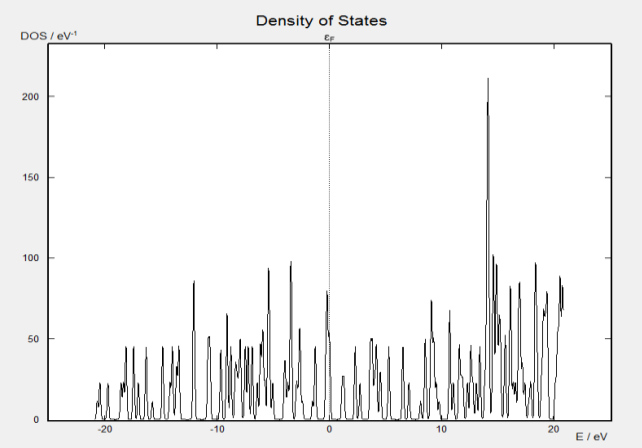


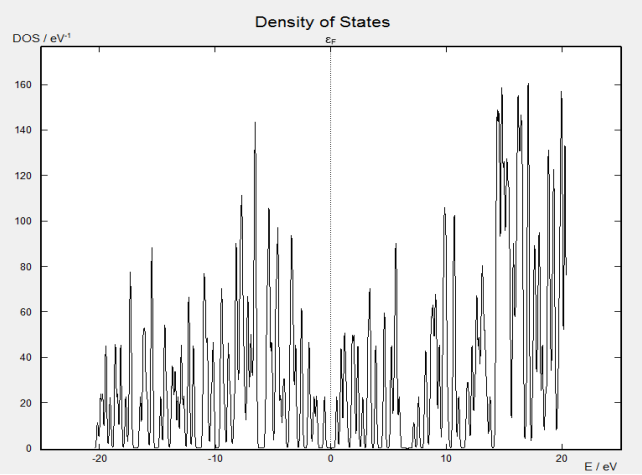
Figure 1. Geometrical structure of (a) (4,1) CNT (b) (4,4) CNT and (c) (4,0) CNT**.**



a)



b)



c)

Figure 2. Density of states (DOS) for (a) (4,1) CNT (b) (4,4) CNT and (c) (4,0) CNT.

The DFT simulation parameters are selected to be the following: mesh cut-off energy is taken as 150 Ry, basis set is double zeta polarized with 0.001 Bohr radial sampling. Brillouin zone integration parameters of electrodes are taken as (1,1,1) and electrode temperature 300 K. These parameters are chosen to provide accurate results as reported earlier.[19] In DFT simulations, the electrodes are assumed to be repeated infinitely in the transport direction and to have bulk-like properties. The length of the electrodes is thus chosen to be sufficiently long to ensure that there is no interaction between the central region and the repeated images of the electrodes. The basis sets used the single-zeta polarized (SZP), and the double-zeta polarized (DZP).[20,21] The DZP is the mostly complete basis set we used, and therefore the one that best predicts the ground state of the system.[21]

To understand the localization of electrons near the Fermi level, we have plotted the density of states profile of the three proposed models using the ATK-DFT. [22] ATK-DFT is based on density functional theory and applies a local atomic orbital (LAO) basis set and Perdew, Burke and Enrzenhofer parameterization of generalized gradient approximation (GGA).[23]The DOS profile of chiral (4,1) CNT is shown in Figure 2(a), whereas the DOS profile of armchair (4,4) CNT and zig-zag (4,0) CNT is shown in Figure 2b and Figure 2c respectively. Figure 2 shows that all these three structures have a distinct DOS in longer energy ranges.

Conclusions

In this study, three SWCNT geometries were simulated using DFT of Atomistic Tool Kit (virtual nanolab) to investigate their distinguishable density of states (DOS) in long energy range. The DOS near the Fermi level in case of chiral and armchair nanotubes are very close to each other which is not the case for zig-zag nanotube. Therefore this study clarifies the theoretical aspects of CNTs so that they can be fully explored in the future electronic industry.

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