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Electronic and Mechanical Properties of (6,1) Carbon nano-tubes with different tube diameter: A Theoretical Studies

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We investigated the electronic and mechanical properties of single-walled carbon nanotubes (SWCNTs) with different tube diameters using density functional theory (DFT) and molecular dynamics (MD) simulation, respectively. The carbon nanotubes' electronic properties were derived from the index number (n_1, n_2), lattice vectors, and the rolled graphene sheet orientation. For (6,1) SWCNT, (n_1-n_2)/3 is non-integer, so the expected characteristic is semiconducting. We have considered (6,1) Chiral SWCNT with different diameters 'd' (4.68 Å, 4.90 Å, 5.14 Å, 5.32 Å, 5.53 Å) corresponds to respective bond-lengths 'δ'(1.32 Å, 1.36 Å, 1.45 Å, 1.50 Å and 1.56 Å) and then analyze the electronic properties from the Linear Combination of Atomic Orbitals (LCAO) based on DFT. We have used both the DFT-1/2 and GGA exchange energy correlation approximations for our calculation and compared the results. In both cases, the energy band gap is decreasing order with the increase in bond lengths. The lowest value of formation energy was obtained at the bond length $\delta = 1.45$ Å ($d = 5.14$ Å). For the mechanical properties, we have calculated Young's Modulus using Molecular Dy-

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namic simulations. From our calculation, we have found that the (6,1) SWCNT with bond length 1.45 Å ($d = 5.14$ Å) has Young's modulus value of 1.553 TPa.

KEYWORDS
Carbon Nanotube,DFT, Band structure, Young's Modulus

1 | INTRODUCTION

Carbon nanotubes (CNTs), which were first experimentally synthesized by Iijima [1] in 1991, have become the focal point of extensive research because of their outstanding electronics [2], mechanical [3] and thermal properties [4]. CNTs with a direct band-gap in the range of ∼1.0 eV, which means they emit light in the near-infrared range [5] is applicable for nano-photonic and nano-telecommunication devices. CNTs have been successfully integrated with other elements for making optoelectronic devices such as detector, LED, field-effect transistor, etc. [6, 7, 8, 9] Pure CNTs exhibit strong absorption and desorption capacity of gases [10, 11, 12]. Based on this, CNTs have become the best choice in making gas sensing detectors. Many researchers have investigated the CNT-based nanocomposites for gas sensing based on different sensing mechanisms [13, 14, 15]. Semiconducting CNTs have superior properties to silicon below 10nm dimension because silicon nano-wire breaks down at around 15 nm[16]. CNTs can be categorized into two types: (i) Single-walled carbon nanotubes (SWCNTs) and (ii) Multi-walled carbon nanotubes (MWCNTs). This categorization is based on wall formation. MWCNTs are cheaper to produce as compared to SWCNT and can be profitably used to make polymer or other composites, enhancing their mechanical, thermal, and electrical properties[17, 18]. Functionalized MWCNTs are highly active catalysts and helps in epoxidation of a wide range of alkenes also functionalization of Multi-Walled Carbon NanoTube (f-MWCNT) greatly affect the rheological properties of water-based drilling muds[19, 20]. Nickel Oxide/CNT Nanocomposites are used for filteration of Cd^{2+} from the Aqueous Solution.[21]. However, SWCNTs have more technological applications due to the presence of finite band gaps[22]. A single-Walled Carbon NanoTube Fragments (SWCNTFs) has been constructed from rolled $C_{102}H_{30}$ graphene sheet that show partial localization of the π electron clouds, enhances strength of Na^{+} interactions. Eventually, improves the surface modification that helps in storage of electric charges by transfer of cations on the surface and may enhanced the hydrogen adsorption capability[23]. A novel catalysts were prepared by holding Cobalt on carbon nanotubes using the wet impregnation method with cobalt loading varying from 15 to 45 wt.%.[24] Also, SWCNTs are more efficient in drug delivery because of their ultra-high surface area and drug-loading capacity [25, 26]. The most exciting characteristic of CNT is the strong dependence of the electronic properties on the tube's geometry. [27] The geometry of an SWCNT is determined by the chiral indices, which are represented by n_1 and n_2 (where n_1 and n_2 are positive integers) [28]. SWCNTs in terms of chirality can be divided into three types which are zigzag (n_1,0), armchair (n_1, n_1),and chiral (n_1, n_2). The SWCNTs are metallic if (n_1-n_2)3 = *integer* or else semiconducting with different size electronic energy gaps [5, 29, 30, 31]. The physical and chemical properties of different SWCNTs have been investigated [32, 33, 34, 35] due to their exotic properties. The electronic structure of 2D [36, 37] and 3D compounds [38] as well as SWCNTs can be modified by controlling the band-gap. Debnarayan et al. [39] calculated the band structures of Boron-Nitrogen doped (8,0) SWCNTs and reported the band-gap change at different concentrations of the dopant atoms. The band-gap can also be controlled by applying stress [40, 41] and electric field [42] as well. Recently,

Patra et al. studied the buckling behavior of non-uniform SWCNT using non-local elasticity theory and the differential transformation method and reported its potential for the development of non-uniform CNT-based devices[43]. Integrated CNTs also possess the potential for building a unified electronic and optoelectronic technology based on the same material. Chena et al.[44] experimentally studied the properties of an intra-molecular p-i-n junction photovoltaic device based on selectively doped SWCNTs. They reported that it behaved as a diode with a high rectification ratio and exhibited a good photovoltaic effect under a 1550-nm monochromatic illustration. Recently, Wang et al. [45] studied the electronic, optical, and mechanical properties of complex one-dimensional material of hydrogenated diamond nano-wires (CNW) encapsulated in (n,n) CNTs (n = 7 to 10) using density functional theory (DFT). They have reported metallicity for the outer CNT and wide band gap semiconducting nature for the inner CNW simultaneously. The values of Young's modulii of the CNW@CNT are 0.996 TPa, 1.015 TPa, 0.992 TPa and 0.980 TPa for (7,7), (8,8), (9,9) and (10,10)-CNT, respectively. The properties mentioned above of a complex structure of CNW@CNT have potential application as a multifunctional in nano-electronics, nano-optoelectronic, and nano-electromechanics. Experimental and theoretical approaches have been developed to characterize SWCNTs' elastic behavior [46, 47, 48]. Discrepancies exist in the experimental measurement of SWCNTs using atomic force microscopy (AFM) and transmission electron microscopy (TEM) with large error bars. Theoretical techniques such as DFT and molecular dynamics (MD) simulation have been routinely applied [49, 50, 51, 52]. A study based on MD simulation on Graphene-based Nano-tubes' mechanical properties [53] and Penta-graphene-based Nano-tubes [54] found mechanical fracture under high strain compared to CNTs due to triple bonds and increased porosity. We have investigated the electronic of (6,1) SWCNT from DFT-based DFT-1/2 and GGA exchange-correlation functionals in our current work. The mechanical properties were investigated using MD Simulations, and we found a high value of young's modulus. The current study provides a theoretical basis for applying (6,1) SWCNT in electronic devices and nano-composites.

2 | COMPUTATIONAL DETAIL

By using a DFT-based computational code VNL-ATK software package [55], we evaluated the (6,1) SWCNT structures with different tube diameters 4.68 Å, 4.90 Å, 5.14 Å, 5.32 Å, 5.53 Å and corresponding bond lengths are 1.32 Å, 1.36 Å, 1.45 Å, 1.50 Å, 1.56 Å. The electronic properties were calculated by using the generalized gradient approximation (GGA) [56] and DFT-1/2 [57]. DFT-1/2 is an application of Slater's half occupation technique designed for enhancing the degenerated energy bandgap. The modified KS potential is $V_{mod-KS}(r)$=V_{KS}(r)-$V_S(r)$, where V_{KS}(r) is a standard DFT potential and $V_S(r)$ is a self-energy potential. The mechanical properties were calculated using MD simulation technique. The MD is a developed method to characterized the effective properties at nano-scale. The Tersoff C 2010 classical potential[58] is used between the carbon atoms. The random initial velocities of the atoms are drawn from the Maxwell Boltzmann distribution corresponding to a temperature of 300K and a series of Molecular dynamic (MD) simulation is performed using ensemble NPT Martyna Tobias Klein algorithm[61]. The time steps of the simulation are set to 200 fs.

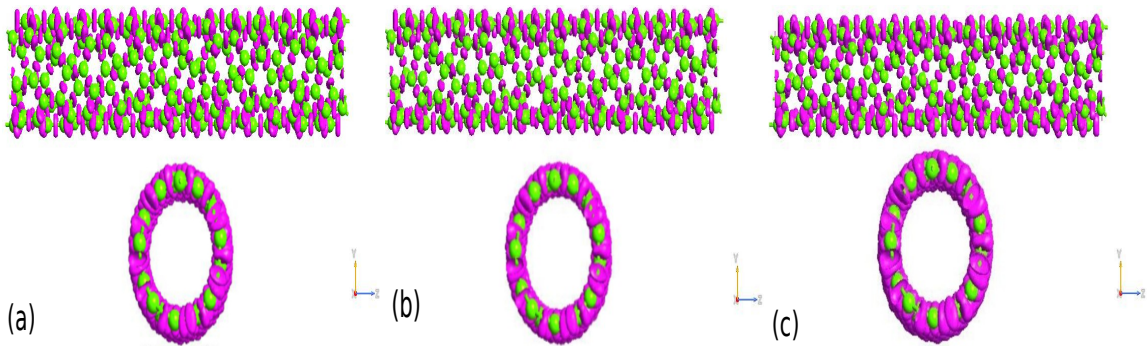

FIGURE 1 . Electron Localization function (ELF) for (6,1) SWCNT calculated form DFT-1/2 for diameter (a) 4.90 Å, (b) 5.14 Å and (c) 5.32 Å

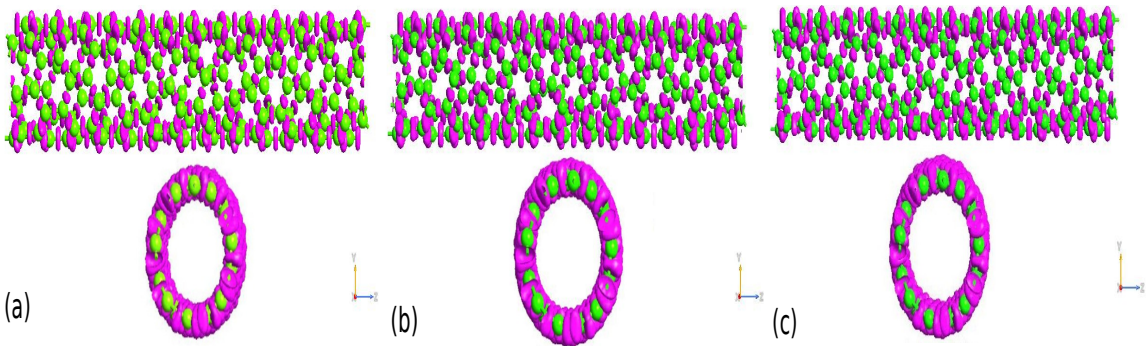

FIGURE 2 Electron Localization function (ELF) for (6,1) SWCNT calculated form GGA for diameter (a) 4.90 Å, (b) 5.14 Å and (c) 5.32 Å

3 | RESULT AND DISCUSSION

In our calculation, we have considered (6,1) Chiral SWCNT with different diameters 'd' (4.68 Å, 4.90 Å, 5.14 Å, 5.32 Å, 5.53 Å) corresponds to respective bond-lengths 'δ'(1.32 Å, 1.36 Å, 1.45 Å, 1.50 Å and 1.56 Å). Among all these CNT, with bond-length δ=1.45 Å is found to be most stable with minimum energy. Further, we have tested the thermodynamical stability by calculating the frequency-dependent phonon-band and phonon-dos for other compressed and stretched CNTs [see Fig. 3]. The presence of positive phonon frequencies in all the considered systems confirm the thermodynamical stability and may be possible to synthesize in lab. The cartesian coordinates for all the system with bond lengths δ'(1.32 Å, 1.36 Å, 1.45 Å, 1.50 Å and 1.56 Å) are given in supporting files.

3.1 | Electronic properties

As reported previously, the semi-empirical tight-binding (TB-π) band model has limitations in estimating the accurate electronic structure for low diameter CNTs (below $d = 6.0$ Å) due to the presence of curvature

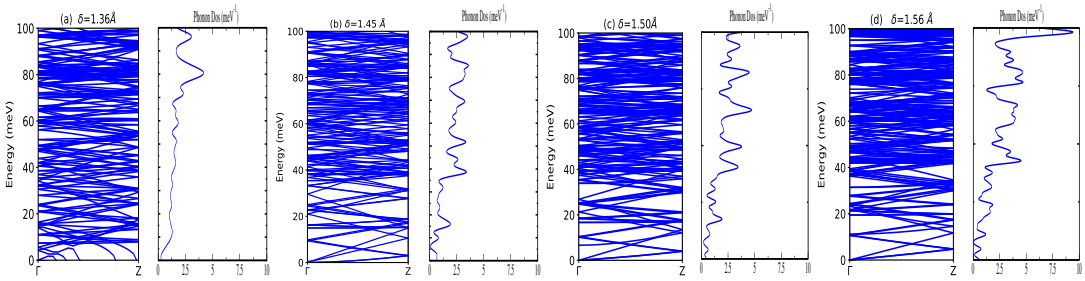

FIGURE 3 . Phonon Band and density of states (phonon-DOS) for (a) δ=1.36 Å, (b) δ=1.45 Å (c) δ=1.50 Å and (d) δ=1.56

effect.[49, 40] We have calculated the electronic band and density of states (DOS) for the optimized CNT by considering three different basis sets viz (a) Linear Combination of Atomic Orbitals (LCAO) (b) Semi-empirical Slater-Koster tight-binding model[59, 60] and (c) DFT Plane-wave (DFT-PW) method[55]. As discussed above semi-empirical tight-binding model is inefficient in analyzing the electronic properties for low diameter CNTs. On the other hand, the DFT-PW method is suitable for small bulk systems, and the physical quantities can be converged systematically. While the DFT-PW method is computationally expensive and inefficient for the nanostructures with large vacuum (open system)[55]. The results obtained from DFT-LCAO, semi-empirical TB model, and DFT-PW is presented in Fig.4(a-c), respectively. We have observed an indirect bandgap of ∼0.345 eV for DFT-LCAO and ∼ 0.412 eV for DFT-PW, while semi-empirical TB does not open the bandgap. DFT-PW method has given a high value of band gap as compared to another basis sets, but this method is computationally very expensive, and convergence in a feasible time is problematic.

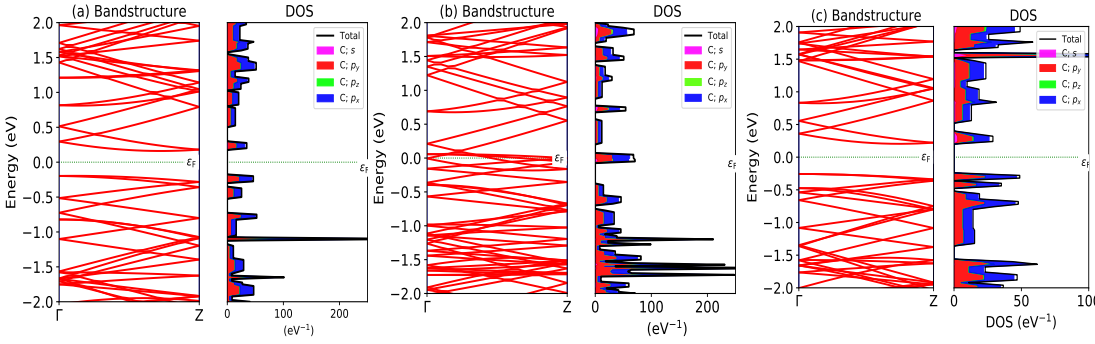

FIGURE 4 . Band structures and density of states (DOS) of optimized CNT calculated from three different basis sets (a) LCAO-DFT (b) TB-Semi-empirical method and (c) Plane Wave method

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Therefore, to obtain the detailed profile of the electronic properties of the (6,1) SWCNT at different bond lengths the electron localization function (ELF), the electronic band structures and density of states (DOS) were calculated using the DFT-1/2 and GGA approximation as implemented in computational package VNL-ATK [55]. Fig(1) and Fig(2) showed the pink-colored solid sphere in between two carbon atoms which is a signature of electron localization, and it is indicative of the covalent bond. The covalent bond arises mainly

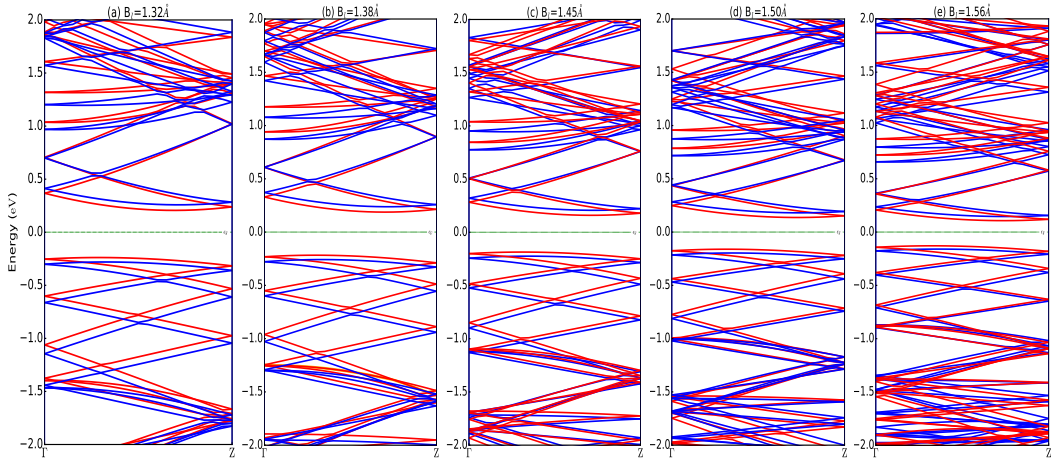

FIGURE 5 . Energy band structure of (6,1) SWCNT Red-GGA and Blue-DFT-1/2 for diameter(bond-length) in Å:(a) d=4.68(δ=1.32), (b)d=4.90(δ=1.38), (c)d=5.14(δ=1.45), (d)d=5.32(δ=1.50) and (e)d=5.53(δ=1.56)

due to the sharing of electrons between p_y-orbitals of C-atoms in-plane direction. On analysis of the band structure and DOS we have found that (6,1) CNT is a semiconductor as expected according to the chiral vector rule $(n_1\text{-}n_2)/3 \neq integer$ [see Fig.(5 and 6)]. The calculated energy bandgap for the (6,1) CNT at different bond lengths using the DFT-1/2 and GGA approximation is presented in Table 1. For all reference bond lengths, the bandgap for DFT-1/2 approximation is larger than the GGA approximation. This is because DFT-1/2 includes the self-corrected Kohn-Sham (KS) eigenvalues from the half-occupied potential of Slater orbital[62] which is missing in GGA approximation. This observation is similar to previous studies [27] where the overall bandgap changed by ∼24.52% with the DFT-1/2 compared to GGA approximation. The result of DFT-1/2 (E_g=0.431 eV) comprehends the band gap (E_g=0.412 eV) calculated from DFT-PW. But DFT-1/2 is computationally much cheaper as compared to DFT-PW. The bandgaps are formed due to the hybridization of $p-p$ orbitals with $\sigma-\sigma$ bond [see Fig.6]. Here we can see the majority contribution from inplane p_y and p_x orbitals of C-atoms (refer to the blue and red lines in Fig.6). In both approximations, the bandgap decreases with an increase in bond length i.e., bandgap decrease with increasing tube diameter. The indirect bandgap lies between Γ and Δ symmetry. The direct bandgap is considered between $\Delta-\Delta$ symmetry. (6,1) SWCNT is a direct bandgap semiconductor along $\Delta-\Delta$ symmetry. Here in Fig.5, Δ lies between Γ and Z symmetries (not shown in the picture). The direct bandgap from DFT-1/2 ranges from 0.316 eV to 0.556 eV as the diameter (d) of the tube decreases from 5.53 to 4.68 Å, whereas using the GGA approximation, the bandgap varies from 0.24 eV to 0.462 eV. Matsuda et al. [63] and Zhonghua et al. [64] also reported the tube diameter and energy bandgap relationship for semiconducting zigzag SWCNTs and semiconducting arm-chair SWCNTs.

To evaluate the relative stability of (6,1) CNT at different bond length, we calculate the formation energy per unit cell which is defined as

$$E_{form} = E_{total} - n \times E_{c-atom} \tag{1}$$

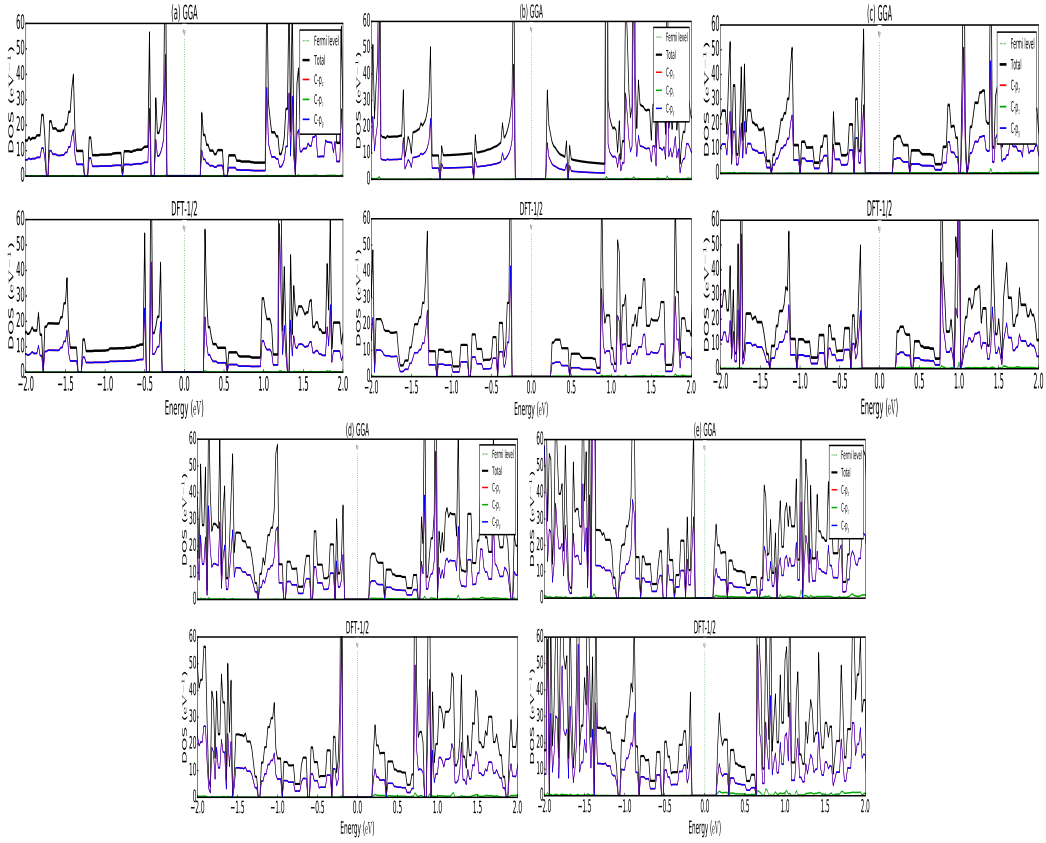

FIGURE 6 . Density of states (DOS) for (6,1) SWCNT calculated from GGA and DFT-1/2 for diameter(bond-length) in Å:(a) d=4.68(δ=1.32), (b)d=4.90(δ=1.38), (c)d=5.14(δ=1.45), (d)d=5.32(δ=1.50) and (e)d=5.53(δ=1.56)

TABLE 1 Bond length δ (Å), tube diameter 'd'(Å), HOMO (E_H), LUMO (E_L), Indirect-bandgap E_{ig} and direct-bandgap E_{dg} calculated from DFT-1/2 and GGA.

bond	tube	DFT-1/2				GGA			
δ(Å)	d(Å)	E_H(ev)	E_L(eV)	E_{ig} (eV)	E_{dg} (eV)	E_H(ev)	E_L(eV)	E_{ig} (eV)	E_{dg} (eV)
1.32	4.68	-0.280	0.258	0.538	0.556	-0.205	0.205	0.411	0.462
1.38	4.90	-0.257	0.238	0.488	0.511	-0.216	0.187	0.404	0.421
1.45	5.14	-0.224	0.206	0.431	0.444	-0.185	0.159	0.345	0.360
1.50	5.32	-0.196	0.180	0.376	0.389	-0.160	0.137	0.297	0.3118
1.56	5.53	-0.159	0.145	0.305	0.316	-0.128	0.107	0.236	0.248

where E_{total} is the total energy of a unit cell, n is the number of carbon atoms in a unit cell and E_{c-atom} is the energy of a carbon atom. Results are summarized in Table2. The formation energies indicate that the considered (6,1) SWCNTs are all energetically stable and the (6,1) SWCNT with bond length of $\delta = 1.45$ Å ($d = 5.14$ Å) having the lowest formation energy.

Tube diameter 'd' (Å)	Bond-length δ (Å)	Formation energy(eV)
4.68	1.32	-7.91
4.90	1.38	-8.36
5.14	1.45	-8.48
5.32	1.50	-8.37
5.53	1.56	-8.12

TABLE 2 Calculated formation energy at for different bond length and tube diameter 'd'

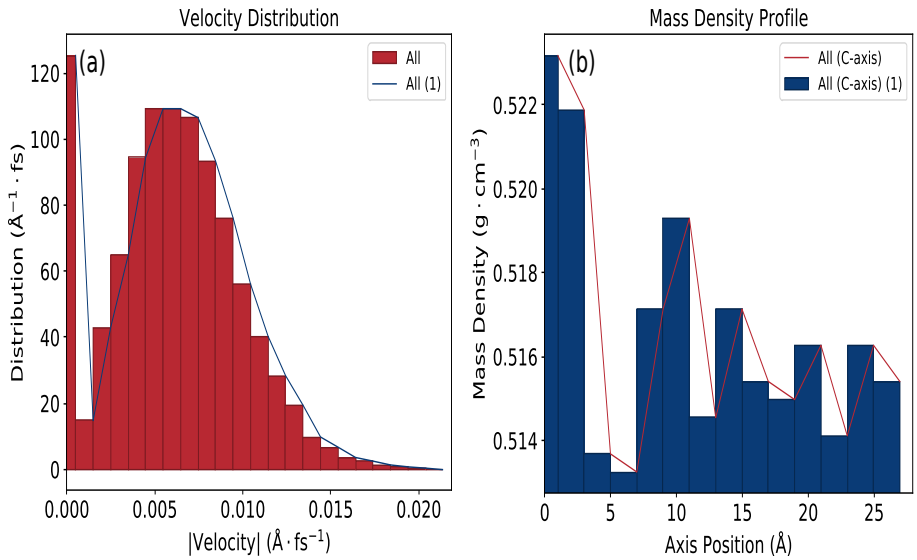

FIGURE 7 (a) Velocity distribution and (b) Mass distribution

3.2 | Mechanical properties

The calculated formation energy showed that (6,1) SWCNT of bond length 1.45 Å has the lowest energy of formation, hence the most stable. A unit cell of (6,1) SWCNT of bond length 1.45 Å is simulated in NPT ensemble at the temperature of 300K and pressure 1 ATM, and a series of MD simulations were performed using the NPT Martyna-Tobias-Klein algorithm [65]. Fig.7(a,b) showed the velocity and mass distribution of the (6,1) SWCNT. Fig.8(a), showed the variation of temperature and potential energy in each time step.

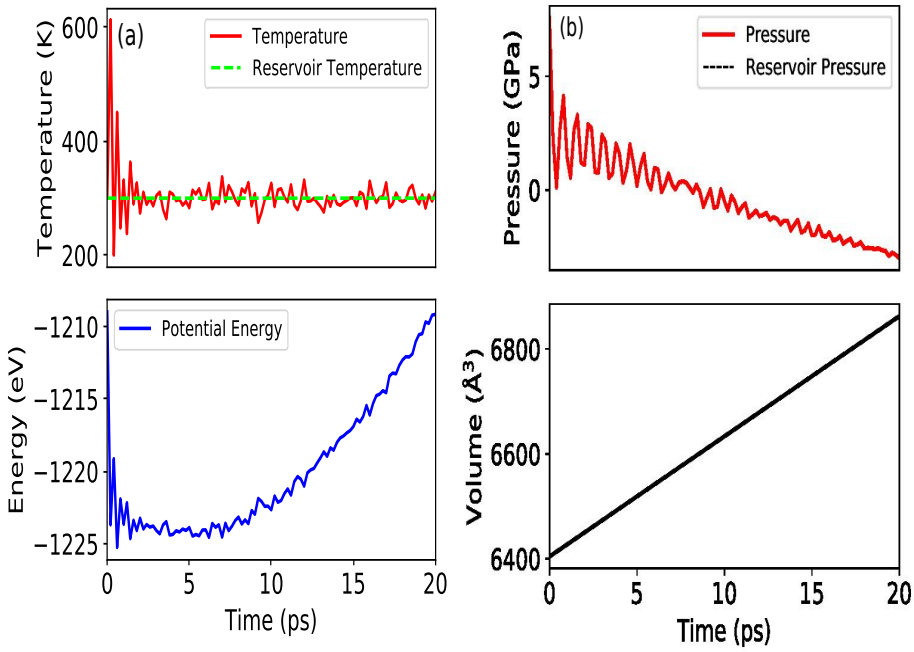

FIGURE 8 (a) Tempetature-Energy and (b) Pressure-Volume values as a function of time steps.

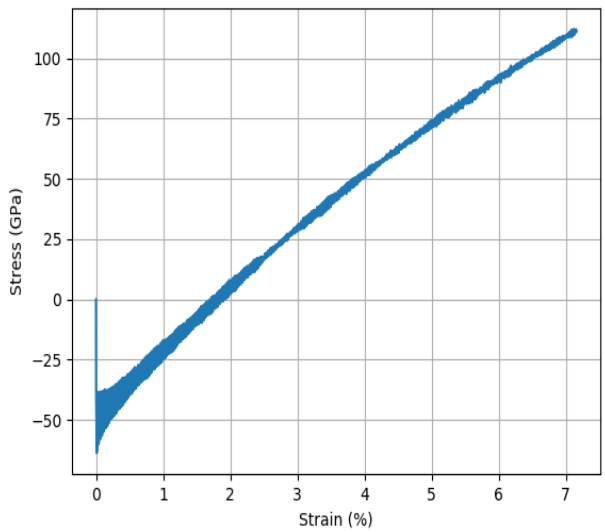

FIGURE 9 Stress-Strain relation in MD simulation

The temperature fluctuates at around 300 K while the potential energy remains negative (below 0 eV). This indicates that the SWCNT is stable and can be realized at room temperature. Meanwhile, Fig.8(b) displays the graph of Pressure-Volume variation with each time step. The pressure fluctuates between 0-5 GPa, and

the volume increases with the time steps. The stress value for each time steps is given by the equation below:

$$\sigma^{\alpha\beta} = 1/V[-\Sigma_i m_i v_i^{\alpha} v_i^{\beta} + 1/2\Sigma_i \Sigma_{j\neq i} F_{ij}^{\alpha} r_{ij}^{\beta}] \quad (2)$$

where m_i and v_i are the mass and velocity of the of the i atom, F_{ij} is the force between i and j atoms, α and β are the Cartesian components, V is the total volume occupied by all the atoms and r_{ij}^{β} is the projection of the inter-atomic distance along the α coordinate [66, 67]. Fig(9) shows the stress and strain relationship for the SWCNT. We found that the simulated SWCNT has a Young's modulus value of 1.553 TPa. This is in good agreement with the previous experimental[68, 69] and theoretical results[70, 71].

4 | CONCLUSION

DFT based on Linear Combination of Atomic Orbitals (LCAO) was carried out to analyze the electronic properties of (6,1) Chiral SWCNT with the following bond lengths: 1.32 Å, 1.36 Å, 1.45 Å, 1.50 Å and 1.56 Å. We have performed the comparative study using two semi-local potentials viz DFT-1/2 and GGA. For the DFT-1/2 and GGA approximations, the energy bands' profile is similar to their energy bandgaps. We have found that the band gap decreases with the increasing bond lengths (tube diameter). For all tube diameters, DFT-1/2 gives a higher bandgap value as compared to GGA. DFT-1/2 increased the overall GGA bandgap by ≈24.52%. The calculated formation energy shows that all the considered structures are energetically stable with minimum energy. Our study (6,1) SWCNT with tube diameter d=5.14 Å (bond length δ= 1.45Å) shows the lowest formation energy. MD-simulation on the (6,1) SWCNT with tube diameter d=5.14 Å (bond length δ= 1.45Å) offers very high stiffness with Young's Modulus value 1.553 TPa.

5 | ACKNOWLEDGEMENTS

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6 | DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

- Y. T. Singh: He is the first author, performing calculations, writing-original draft, writing-review & editing.
- P. K. Patra: Conceptualization, date curation, formal analysis.
- K. O. Obodo: Formal analysis, data curation, investigation.
- D. P. Rai: Methodology, Resources, Licensed software (VNL-ATK), supervision, validation, Result analy-

sis, visualization, validation, final compilation of paper.

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Conflicts of interest/Competing interests

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