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

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April 23, 2021

Abstract

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 a 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 δ = 1.45 Å (d = 5.14 Å). For the mechanical properties, we have calculated Young's Modulus using Molecular Dynamic 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.

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