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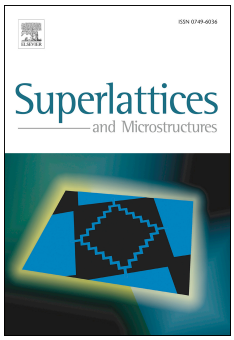

Structural parameters, electronic properties, and band gaps of a single walled carbon nanotube: A p_Z orbital tight binding study

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Structural parameters, electronic properties, and band gaps of a single walled carbon nanotube: A p_z orbital tight binding study

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Abstract

Single walled carbon nanotube (SWCNT), an emerging one-dimensional carbon nanostructure, have several unique attributes and amazing properties that offers a great potential for interconnects, nanoelectronic and optoelectronic devices. For the first time, the p_z orbital tight binding study on structural parameters, electronic properties, and band gaps of a SWCNT have been presented and analyzed in this paper. The analytical values of different parameters regarding the overall unit cell and molecular structure of a SWCNT have been verified using the simulation approach, therefore, proved the validation of both the simulation as well as analytical values. It has been observed that the total number of unit cells, carbon atoms, and hexagons within the overall unit cell and molecular structure of a SWCNT at different chirality values and lengths obtained using the simulation matches with the analytical values. Further, the metallic and semiconducting properties of a SWCNT can be investigated with the help of different simulated electronic band structures obtained for different chirality combinations. First, it has been found that all armchair SWCNTs are metallic with a very small constant band gap of 10.88meV whereas the zigzag SWCNTs show metallic as well as semiconductor behavior with zero and larger than zero band gap values. Second, it has been observed that the total number of subbands in each electronic band structure of a SWCNT (both armchair and zigzag) is chirality dependent and equal to the total number of carbon atoms present in their overall unit cell structure. Furthermore, the reported band gap values have been compared with the already published calculation as well as experimental values which show excellent agreement between them. Finally, it has been observed that the