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Thermodynamic Analysis on the Computationally Designed Single-Walled Carbon Nanotubes †

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Abstract: The Carbon Nanotubes (CNTs) are the novel graphene structure that exists in cylindrical shapes. Usually, the molecules in CNTs consist of the rolled-up single-layer graphene sheet. It includes the Single-Walled Carbon Nanotubes (SWCNTs) with a diameter of less than 1 nanometre (nm) and Multi-Walled Carbon Nanotubes (MWCNTs) with diameters more than 100 nm, which are distinguished by their number of layers. The length of these CNTs can reach up to several micrometers or even millimeters as well. The mechanical and thermal properties of CNTs play an important role in analyzing their unique structure and shapes. Because of these significant thermal and mechanical properties, the carbon nanotubes can be identified as the ideal material to perform the scientific study on low dimensional phonon physics and thermal management at micro and macro scales. In this study, we started to explore the thermal properties of carbon nanotubes (CNTs) by measuring the effective thermodynamic properties like specific heat and thermal conductivity for the bulk samples of Single-Walled Carbon Nanotubes (SWCNTs). As we know that in this modern era, the Carbon Nanotubes (CNTs) are represented as a revolutionary change in the field of nanoscience and nanotechnology; therefore, it is important to understand the basic nature with mechanical and thermal properties of these carbon nanotubes (CNTs) along with their applications including construction process. Hence, we have designed/constructed the single-walled carbon nanotubes (SWCNTs) with different dimensions by employing open-source software like LAMMPS, GROMACS, and AVOGADRO. Further, we computed the thermodynamic properties (i.e., specific heat and thermal conductivity) of these designed/constructed SWNTs by using LAMMPS for different orientations to analyze them more significantly. The predicted basic results of this study are quite interesting and consistent with the literature.

Keywords: nanotechnology; carbon nanotube; SWNTs.

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Conflicts of Interest

The authors declare no conflict of interest.