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Comparison of the electrical properties between pure and impure single-walled carbon nanotubes through molecular simulation modeling

Single-walled carbon nanotubes (SWCNTs) represent a structure of great interest due to their outstanding mechanical and electrical properties since its discovery in 1991. The ability to manipulate SWCNTs to generate metallic or semiconducting structures is invaluable for applications such as nano-transistors. Nevertheless, different methods employed to synthesize these structures caused impurities in the SWCNT structure, which in turn may hinder its electrical characteristics when compared to purified SWCNTs.

As a result, the focus of this preliminary study is to simulate through molecular dynamic modeling using Gaussian03™ the energy dispersion of purified and non-purified SWCNTs. Both types of structures are compared in terms of their energy dispersion through the band structure and the energy density of states. The electrical characteristics of pure SWCNTs have already been identified by previous research work. Therefore, the non-purified models will be compared to these pure structures so as to quantify the effects of these changes in the chemical composition of the nanotube structures.