

# Study of defects in carbon nanotubes produced by ionizing radiation

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The effect of the ionizing radiation on the structure and properties of Carbon Nanotubes (CNTs) is of great theoretical and practical interest, due to their potential applications in the electronics and other fields, including nuclear energy. Although several investigations have been devoted to this issue in the last years [1-5], many aspects of that interaction are still not well understood. With the objective of achieving a better understanding of these processes, in the present work the Density Functional based Tight Binding method (DFTB) is used to study CNTs of single and multiple layers, in which the kind of defects that typically appear under the action of the radiation (vacancies, divacancies, Stone-Wales defects and other) were introduced. The results related with the energy of formation of those defects and the geometric and energy modifications that take place in the CNTs with different chirality and number of layers are presented.

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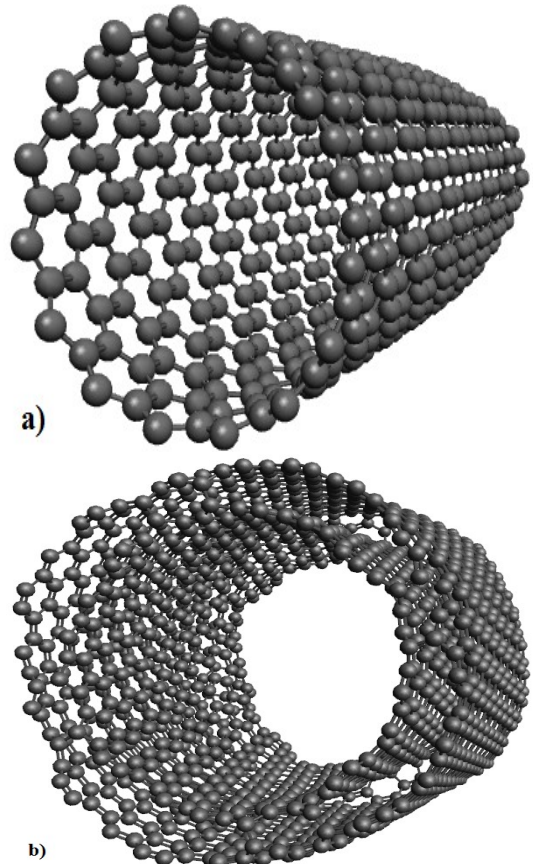


Figure 1: Optimized geometries using DFTB. a) Single layer zigzag nanotube (15,0) and length 3.5 nm b) Double layer chiral nanotube (7,13)(8,20) and length 2.5 nm.