

Abstract Submitted  
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**Fullerene and Carbon Nano Tube for Cancer Treatment** JUNG EUN BYUN, ISAAC KIM, RICHARD KYUNG, Choice Research Group — A molecule or compound becomes reactive after it gives off electrons by the molecular dynamics. This helps to stabilize the cell affected by cancer caused by the Reactive Oxidative Species (ROS). This project aims to determine the thermodynamic stability of various compounds in Fullerene, carbon nano tubes and their derivatives using a computational quantum physics and chemical physics. Density Functional Theory (DFT) and molecular mechanics are used in order to model the electron properties of the compound. Through the simulation, better and safer functional groups with fullerene, which can be used in the cancer treatment with less optimization energy, were found by checking their optimized molecular energy both stereo-chemically and thermo-dynamically. Using the Avogadro and Gamess that allow performing such computations for the compounds, this program shows the optimized geometry energy levels of Fullerene Nano Molecules Used in PDT (Photodynamic Therapy) and fully determines the theoretical values of the structures atomic properties.

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