

Abstract Submitted
for the TSF19 Meeting of
The American Physical Society

Study on the Nanoparticles Used in Treatment for Cancer Using Bio-chemical and Computational Analysis NUO CHENG, RICHARD KYUNG, CRG-NJ — Computational biomedical simulation with nano technology is perceived as a new approach to an alternative method for future solution of cancer research. In recent years, potential solutions in cancer treatment used nano scaled carbon nanotube complexes, since they are believed to be able to stabilize the cells affected by cancer. A free-radical chain reaction capable of propagating in space is the major oxidative reaction in biomembranes. In the light of the promising use of carbon nanotube complexes, this paper studies their thermodynamic safety and stability to inhibit the free-radical chain reaction which propagates in tissue space. For this purpose, we used the program Avogadro to model, optimize, and compare the resulting molecular energy of the clusters. Various types of Carbon Nanotube(CNT) derivatives were tested for their thermodynamic stabilities, which were measured through the optimized energies. The reactivity and conductivity were also measured through the dipole moments to calculate the activity level the molecule could have with other nearby molecules. Lastly, electrostatic potential maps were utilized to visualize the polarization and assess the reactivity level of each molecule.

Richard Kyung
CRG-NJ

Date submitted: 20 Sep 2019

Electronic form version 1.4