

Abstract Submitted
for the NES19 Meeting of
The American Physical Society

Biochemical and Thermodynamic Analysis of the Nano-scaled Molecules in the Treatment of Tumor Cell Affected by ROS ISABELLA BAEK, Northfield Mount Hermon, HAYOUNG KYUNG, Harvard University — Multiple pathways through oxidative stress due to Reactive Oxygen Species(ROS) can cause cell injury and cancer. Computational biomedical simulation technology is perceived as a means of new approach to an alternative method for future solution of cancer research. In recent years, potential solutions in applications-related nano technology use nano-scaled fullerene complexes, as they are believed to be able to virtually attach large quantity of protons and can act as electron donors. In the light of the promising use of fullerene complexes, current study conducted their biochemical and thermodynamic analysis of the nano-scaled molecules. In this paper, the molecular energy of fullerenes doped with clusters such as hydroxyl(OH), carboxyl(COOH), and malonic acid(C-COOH) derivatives, was measured first. And then, comparisons of the BB types of derivatives such as BB7, BB8, and BB9 on C40 and C72 fullerene models were made. It was observed that C72 derivatives had much lower optimization energy levels (kJ/mol) than those of C40. The softwares Avogadro and Chemcraft are open-source molecular editing program equipped with an auto-optimization feature, which determines the theoretical values of a certain structures atomic properties through the Density Functional Theory (DFT).

Richard Kyung
Choice Research Group

Date submitted: 14 Mar 2019

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