

Abstract Submitted
for the NES17 Meeting of
The American Physical Society

Nano Particles and Fullerene Derivatives Used in Reduction of ROS in Cancer Treatment YONGWOO LIM, Pomfret School, RICHARD KYUNG, Choice Research Group — Certain reactive oxygen species in the human body can cause oxidative stress to biological cells due to the process of uncontrolled radical reactions. Methods of using fullerenes to control reactions were researched to determine whether or not fullerenes are apt for cancer treatments. Gamess, Avogadro and Chemcraft molecule simulators were used to measure the optimized energy and electrostatic forces acting on the fullerenes when they are attached with hydroxyl, carboxyl groups and other functional groups; and through this, analysis of the thermodynamic stability was conducted. Experimental results also proved that C60 were the most effective in reducing oxygen radicals because chemiluminescence times were the shortest out of all the test subjects. Through the simulation of several different fullerenes, those with lower enthalpies with chemical stability that is suitable for medical use were found. Although fullerene such as C40 had decreasing enthalpies when combined with hydroxyl and carboxyl groups, it had higher enthalpies ranging from 24,000 to 27,000 kilojoules per mole. Fullerene such as one of C82 isomers was more viable as it had a significantly lower range of 11,000 to 17,000 kilojoules per mole even though its enthalpies increased when combined with other groups.

Richard Kyung
None

Date submitted: 17 Mar 2017

Electronic form version 1.4