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Assessment of Thermodynamic Properties of Carbon Nanotubes(CNTs) and Hydrated C60 Fullerenes(C60HyFn) as Potential Agents to Suppress Reactive Oxygen Species CHRISTY YOON, RICHARD KYUNG, Choice Research Group — Oxidation of the neural tissues in human brain causes neurodegenerative disease; however, information on the sub-cellular localization of oxidative molecules is not provided in detail thus far. It is highly desirable to visualize the activities of Reactive Oxygen Species (ROS) in living cells on a microscopic level for the proper mechanism of the role of peroxidation. Multiple pathways through oxidative stress can produce cell injury; and thus, the oxidative reactions in biomembranes are particularly important. It can result in the impairment of lipidprotein interaction and modification and fragmentation of membrane proteins as well, thereby leading to the cell injury and aging. A free-radical chain reaction capable of propagating in space is the major oxidative reaction in biomembranes. In this paper, the functionalized Carbon Nanotubes(CNTs) and hydrated C60 Fullerenes(C60HyFn) molecules were thermodynamically studied to determine whether the molecules stabilize or destabilize the molecules. The Auto Optimize Tool in the computational software was used for each Carbon Nanotubes(CNTs) and hydrated C60 Fullerenes(C60HyFn) derivatives modeled in this project to determine its optimization energy. The Universal Force Field (UFF) option was selected for all the molecules modeled.

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