Giant Fullerenes for Target Specific Drug Delivery\textsuperscript{1} ROBERT COURTNEY, BORIS KIEFER, New Mexico State University — Carbon nanostructures, such as giant fullerenes, have a great potential for biological and medical applications. Most of the previous research is dedicated to investigate the use of fullerenes as vehicles for carrying medication which is chemisorbed on the outside surface of the fullerenes. In contrast, using fullerenes as an enclosure was largely abandoned due to the high strength of the carbon-carbon bonds which has been perceived to prevent the rupturing of the fullerene to release their cargo. We performed atomistic computations based on classical force fields that will address this perception. Specifically we explore the physics and chemistry of OH functionalized carbon based giant fullerenes with diameters from 0.72 nm (60 atoms) to 5.7 nm (3840 atoms). The preliminary results show that OH functionalization on these fullerenes is not only viable but also provides a pH sensitive release mechanism. Furthermore our current results show that carbon-carbon bonds can be broken in low energy biological environments in the presence of a flow induced strain field. These insights may have implications for target specific drug delivery in general and cancer treatment in particular.

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