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Mathematical Model for Interaction Energy of Toroidal Molecules and Other Nanostructures

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Abstract : Carbon nanotori provide several properties such as high tensile strength and heat resistance. They are promised to be ideal structures for encapsulation, and their encapsulation ability can be determined by the interaction energy between the carbon nanotori and the encapsulated nanostructures. Such interaction energy is evaluated using Lennard-Jones potential and continuum approximation. Here, four problems relating to toroidal molecules are determined in order to find the most stable configuration. Firstly, the interaction energy between a carbon nanotorus and an atom is examined. The second problem relates to the energy of a fullerene encapsulated inside a carbon nanotorus. Next, the interaction energy between two symmetrically situated and parallel nanotori is considered. Finally, the classical mechanics is applied to model the interaction energy between the toroidal structure of cyclodextrin and the spherical DNA molecules. These mathematical models might be exploited to study a number of promising devices for future developments in bio and nanotechnology.

Keywords : carbon nanotori, continuum approximation, interaction energy, Lennard-Jones potential, nanotechnology
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