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Drug Delivery of Cyclophosphamide Functionalized Zigzag (8,0) CNT, Armchair (4,4) CNT, and Nanocone Complexes in Water

Authors : Morteza Keshavarz

Abstract : In this work, using density functional theory (DFT) thermodynamic stability and quantum molecular descriptors of cyclophoshphamide (an anticancer drug)-functionalized zigzag (8,0) CNT, armchair (4,4) CNT and nanocone complexes in water, for two attachment namely the sidewall and tip, is considered. Calculation of the total electronic energy (Et) and binding energy (Eb) of all complexes indicates that the most thermodynamic stability belongs to the sidewall-attachment of cyclophosphamide into functional nanocone. On the other hand, results from chemical hardness show that drug-functionalized zigzag (8,0) and armchair (4,4) complexes in the tip-attachment configuration possess the smallest and greatest chemical hardness, respectively. By computing the solvation energy, it is found that the solution of the drug and all complexes are spontaneous in water. Furthermore, chirality, type of nanovector (nanotube or nanocone), or attachment configuration have no effects on solvation energy of complexes.

Keywords : carbon nanotube, drug delivery, cyclophosphamide drug, density functional theory (DFT)
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