

576g Interaction between DNA Molecules and Fullerenes: Molecular Dynamics Study

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Atomistic molecular dynamics simulations are performed for up to 20 nanoseconds to monitor the formation and the stability of complexes composed of single or double strand DNA molecules and C60 in aqueous solution. Despite the hydrophobic nature of C60, our results show that fullerenes strongly bind to nucleotides. The binding energies are in the range -22 to -47 kcal/mol; by contrast, the binding energy of two fullerenes in aqueous solution is only -7.5 kcal/mol. We observe the displacement of water molecules from the region between the nucleotides and the fullerenes and we attribute the large favorable interaction energies to hydrophobic interactions. The features of the DNA-C60 complexes depend on the nature of the nucleotides: C60 binds to double-strand DNA, either at the hydrophobic ends or at the minor groove of the nucleotide. C60 binds to single-strand DNA and deforms the nucleotides significantly. Unexpectedly, when the double strand DNA is in the A-form, fullerenes penetrate into the double helix from the end, form stable hybrids, and frustrate the hydrogen bonds between end group base pairs in the nucleotide. When the DNA molecule is damaged (specifically, a piece of nucleotides consisting of four bases removed), fullerenes can stably occupy the damaged site. We speculate that this strong association may negatively impact the self-repairing process of the double strand DNA. Our results clearly indicate that the association between C60 and DNA is stronger and more favorable than that between two C60 molecules in water. Therefore our simulation results suggest that C60 molecules have potentially negative impact on the structure, stability, and biological functions of DNA molecules.