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Molecular Dynamics Studies of RNA Nanotubes

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RNA molecules are very flexible in nature. This feature allows us to build various motifs which are essential in bio-nanotechnological applications. Based on the previous studies on RNA nanorings [1, 2], in this contribution we analyze the structure and properties of RNA nanotubes, where we focus on nanotubes consisting of up to five nanorings of around 20nm in diameter. We have developed a molecular dynamics (MD) method and implemented it by using the NAMD and VMD packages to study the structural and thermal properties of the nanotube in physiological solutions. In particular, we have analyzed such characteristics as the Root Mean Square Deviation (RMSD), the radius of gyration, the number of hydrogen bonds per base pairs, and the radial distribution function for the different nanoclusters in nanotubes of various sizes. The variations of energy and temperature with simulation time have been studied for all sets of simulations. Variations in RMSD, radius of gyration and the radial distribution function with temperature have been analyzed in detail. Furthermore, the number of $^{23}Na^{+}$ ions around the nanotubes within the distance of 5A at two different temperatures has also been studied. It has been found that the number of ions accumulated around the nanotubes within the specified distance is growing with increase in temperature from 310K to 510K. The final configurations of the systems simulated at 510K have been considered as the starting point for further MD simulations at 310K. We confirmed the process of ion evaporation with temperature decrease. This is due to the phenomenon of self-stabilization, first reported in [2].

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