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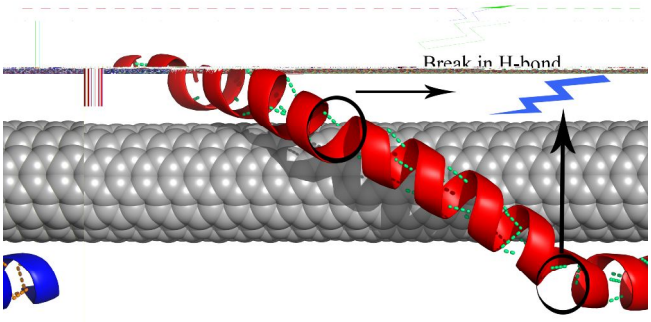
Exploring the Changes in the Structure of α-Helical Peptides Adsorbed on to Single Walled Carbon Nanotube Using Classical Molecular Dynamics Simulation

Classical molecular dynamics (MD) simulation has been carried out in explicit solvent environment to understand the interaction between single walled carbon nanotube (SWCNT) and α-helix. A polyalanine peptide composed of forty alanine residues has been chosen as the model for α-helix (PA_{40}). Results reveal that SWCNT induces conformational changes in PA_{40}. Furthermore, breakage of hydrogen bonds in the chosen model peptides has been observed which leads to conformational transitions (α → turns) in different parts of the PA_{40}. Owing to these transitions, regions of different structural and energetic stability are generated in PA_{40} which enable the PA_{40} to curl around the surface of SWCNT. The overall observations obtained from MD simulation are not significantly influenced by the starting geometry and the choice of the force field. Evidences from MD simulation on the interaction of α-helical fragment of the SNARES protein with SWCNT elicit that the amino acid composition influences the interaction pattern. However, the wrapping of α-helical fragment of the SNARES on to SWCNT is similar to that of PA_{40}. Overall there is a considerable decrease in the helical content of peptides upon interaction with SWCNT in agreement with the experimental findings. In addition to this. a systematic molecular dynamics (MD) simulations of PA_{40} with SWCNTS of different chiralities, *i.e* (6,6), (10,10), (14,14), (18,18) and graphene sheet have been carried out to unravel the relationship between the curvature and the helix breaking tendency of the carbon nanomaterails. It is found that the decrease in the helical content is inversely proportional to the curvature of the nanomaterails.



Reference

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