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Structure and Properties of HELICAL CARBON NANOTUBES through MD Simulations. AKSHAY DAHIYA, Department of Mechanical Engineering, Indian Institute of Technology Ropar, DEEPTI VERMA, Chemical Engineering and Materials Science Department, University of Minnesota, SHAKTI S GUPTA, Department of Mechanical Engineering, Indian Institute of Technology Kanpur — Helical Carbon Nanotubes (HCNTs) are coiled 3-valent carbon networks which represent pure carbon helix. Here we study the geometries of two classes: hexagonal helix containing purely polyhex networks and the second class with 5-and 7-membered rings besides hexagons. We followed a model of hexagonal, single wall HCNTs, and determined their relaxed configuration using MD simulations based on Tersoff potential. A race-track like structure is observed in the cross-section of HCNTs upon minimization. For generating class two helix, the adjacency matrix eigenvector's (AME) method is applied which utilizes 3-coordinated tiling of the plane by 5-,6-,and 7-membered ring for the construction of helical structures. The application of the AME method to torusenes is crucial for class two helix generation as it is based on an appropriate choice of bi-lobial eigenvectors triplet which can be selected on the basis of their nodal properties as verified here. After 3-D transformations the final structure was obtained with the help of MM3-potential based MD simulations on Tinker commercial code. The spring constants of HCNTs are computed through MD simulations.

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