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Structure of a DNA-carbon nanotube hybrid using replica exchange molecular dynamics[1] ROBERT JOHNSON, A.T. CHARLIE JOHNSON, MICHAEL KLEIN, University of Pennsylvania — DNA-carbon nanotube hybrids (DNA-CN) are novel nanoscale materials that consist of single-wall carbon nanotubes coated with a self-assembled monolayer of single stranded DNA (ssDNA). Many recent experiments have demonstrated that this nanomaterial is an ideal candidate for a variety of nanotechnological applications. Despite the importance of this material, a complete understanding of its structural and physical properties is lacking. Recent molecular dynamics (MD) simulations of this nanomaterial have provided information about the self-assembly mechanisms and possible ssDNA conformations that characterize DNA-CN. However, MD simulations of biopolymers at low temperatures (T $\sim$ 300 K) result in kinetic trapping and limits sampling of ssDNA configurational space. Here, we present the results of large scale replica exchange molecular dynamics simulations that provide robust sampling of the multitude of ssDNA conformations about SWCN.

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