METRICS FOR THE STUDY OF DNA–CNT HYBRIDS

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DNA-carbon nanotube (DNA-CNT) hybrids have many useful properties important in the field of nanoscience. Molecular dynamics simulations are well-suited to provide insights into the fundamental properties of DNA-CNT hybrids because they enable calculation of structural properties with atomic resolution. Radial distribution functions are often used to detect structural properties of liquids and crystalline materials in MD simulations. In this work other metrics for measuring how well ss-DNA conforms onto CNT were defined, tested, and compared to radial distribution functions. Three measures were defined as the maximum, minimum and average of the point-to-set distances intended to measure how close and tight the ss-DNA wraps around the CNT. An axial distribution function with respect to the z-axis was also defined. It is based on an expanding cylinder centered in the symmetry axis of the CNT instead. A simple ss-DNA (Poly-C) was used for testing purposes. A complex process of model building, simulation and data analysis was completely automated as a script (MoSDAS). Simulations were performed for Poly-C's with varying number of bases. Both of the metrics defined above as well as two radial distribution functions provided by the GROMACS MD package were compared. It was found that MoSDAS greatly simplifies the simulation process and avoids errors. Also, the point-to-set based metrics provides better information than the other measures on when the ss-DNA wraps around the CNT. The axial distribution function was best suited as an indicator of how the DNA atoms conform around the CNT. Analysis of this function shows, for example, a shift to larger CNT-DNA distances as the ss-DNA length increased. A two-peak distribution suggests that different parts of the Poly-C agglomerate at different levels. This information is not evident in the usual radial distribution functions.