COMPUTATIONAL TOOLS FOR THE STUDY OF INTERACTIONS BETWEEN ss-DNA and CNT

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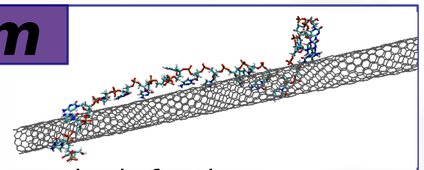
Problem

Molecular Dynamics Simulations

Based on the interactions between a single stranded DNA (ss-DNA) and a single walled carbon nanotube (CNT).



To develop methods for the automation of the simulations of Poly-C ss-DNA of different lengths adsorbing to a CNT.

To develop metrics for the measuring of the distances between the ss-DNA and the CNT.

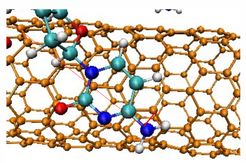
Procedure

- Development of the Model building, Simulation and Data Analysis Script (MoSDAS) to automate the production of the complete system.
- Performed molecular dynamics simulations using the GROMCS MD package.
- Development of a computer program based on the measurements of the Minkowski distance.
- Used of the radial distribution function program of the GROMACS MD package to measure the distances w/r to the CNT atoms and w/r to the center of mass of the CNT.
- Development of a computer program to measure the axial distribution of the atoms with respect to the z-axis.
- Determined which metric its the best for analyzing the data.

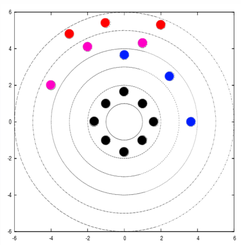
Metrics

Minkowsky Distances Graph (MDG)

Maximum, average and minimum Minkowsky distances between one atom in each of the Poly-C rings and the CNT during the simulation.



Probability Distribution Functions



Axial w/r to z-axis, Radial w/r to one atom and Radial w/r to many atoms. They are based on an expanding cylynder, an expanding sphere and many spanding spheres respectively.

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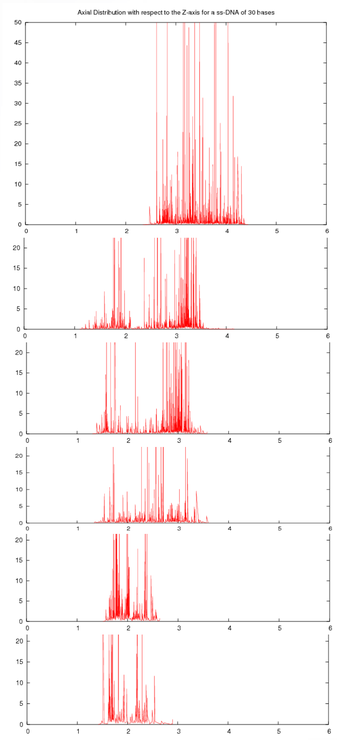
Results and Conclusions



Axial Probability Distribution Functions (APDF)

The APDFs graphs (left) show the distribution of the atoms in the ss-DNA w/r to the z-axis for ss-DNAs of 5, 10, 15, 19, 25 and 30 monomers. Agglomerations of atoms at different levels are observed for some molecules. They also show a shift to larger CNT-DNA distances as the ss-DNA length increased.

Radial Probability Functions (RPDF)

RPDFs of ss-DNA atoms w/r to the CNT atoms and w/r to the center of mass of the CNT (top right) are from (15)Poly-C. They are similar to the RPDF's of Polt-C's of length 5, 10, 19, 25 and 30 (not shown).

Minkowsky Distance Graph

MDG for (30)Poly-C (bottom right) shows when the ss-DNA wraps completely around the CNT.

Conclusions

The MoSDAS greatly simplifies and avoids errors in the simulation process. The APDF and the MDG give more significant information about this particular simulation than the RPDF's provided by the GROMACS MD package.