Molecular Dynamics Simulations of ss-DNA conformation about Carbon Nanotubes

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DNA-Functionalized Carbon Nanotube Chemical Sensors

http://www.lrsm.upenn.edu/~nanophys/biosensors.html
Carbon Nanotubes

- Carbon nanotubes are cylindrical sheets of carbon that were discovered in 1991.

- Nanotubes have diameters of about 1 nm and lengths up to a few centimeters.

- Nanotubes have been a popular subject for condensed matter physics research as well as a top candidate for applications in nanotechnology.
A Single-stranded DNA (ss-DNA) is a DNA molecule consisting of only one chain of alternating sugars and phosphates.

Examples:

- A form
- B form
Problem

To develop methods for automatically Molecular Dynamics Simulations of Poly-C ss-DNA of different lengths adsorbing to Carbon Nanotubes.
Initial Setup

- Ions
- Straight Poly C ss-DNA
- Infinite CNT
- Water
Poly C straight ss-DNA

B form

<table>
<thead>
<tr>
<th>Angles</th>
<th>B-Form</th>
<th>Straight Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>-46.1</td>
<td>161.0</td>
</tr>
<tr>
<td>β</td>
<td>-146.5</td>
<td>-289.0</td>
</tr>
<tr>
<td>γ</td>
<td>36.4</td>
<td>53.0</td>
</tr>
<tr>
<td>δ</td>
<td>156.5</td>
<td>202.0</td>
</tr>
<tr>
<td>ε</td>
<td>154.7</td>
<td>298.0</td>
</tr>
<tr>
<td>ζ</td>
<td>-95.6</td>
<td>-51.0</td>
</tr>
<tr>
<td>η</td>
<td>-97.8</td>
<td>-141.0</td>
</tr>
</tbody>
</table>

Straight form
Backbone torsion angles

Example: $\alpha$ angle

Reference plane

Angle forming bond
**Description of procedure**

- Generate a ss-DNA of Poly C with straight conformation using **nucleic.x** (modified by us).
- Set up system with Poly-C, nanotube, solvent and ions.
- Generate the files required by the simulator.
- Run the molecular dynamics simulation via **mdrun_mpi**.
- Analyse the data produced by the simulation.

This procedure is currently being automatized. Some editing steps require new programming in order to avoid manual manipulation of the system.
Preliminary results
Measurement of the distance
Data analysis

Poly-C with 10 bases suggests stabilization after time.

Poly-C with 25 bases does not show stabilization after 30 times the amount of time.
Acknowledgments

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Questions??
Potential

Distance between atoms i and j

\[ U(r_{ij}, \theta_{ijk}, \phi_{ijkl}) = K_C r (e^{-\gamma(r_{ij}-r_C)} - 1)^2 + \frac{1}{2} K_C \theta (\cos \theta_{ijk} - \cos \theta_C)^2 \]

\[ + \frac{1}{2} K_C \phi (1 - \cos 2\phi_{ijkl}) + 4\epsilon_C C \left[ \left( \frac{\sigma_{CC}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{CC}}{r_{ij}} \right)^{6} \right], \]

Bond term

Bending term

Bending angle

Torsion angle

Torsion term

Van der Waals term