



"Soft-Matter Seminar"

DNA, siRNA mechanics and interaction with Carbon nanotubes

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Abstract

Using fully atomistic molecular dynamics (MD) simulations, we study the dsDNA overstretching and unzipping transition and interaction of dsDNA/small interfering RNA (siRNA) with Carbon nanotubes. We obtain the force-extension curves at various temperatures in constant-force ensemble at different pulling rates viz., 10^{-4} – 10^{-6} pN/fs. Associating the force dependent Gibb's free energy changes to the thermal melting studies, we obtain the overstretching phase diagram. In the next part, I will discuss siRNA molecule wrapping through unzipping on Carbon nanotube and translocation inside nanotube. The siRNA wrapping via unzipping and translocation were initiated and driven by van der Waals interaction between the aromatic rings of siRNA and CNT surface that was facilitated by the two sticky ends on both strands of siRNA. The adsorbed and translocated siRNA complex remains stable over the entire duration of simulation (~ 50 ns long). However dsDNA of the same sequence cannot unzip and wrap around nanotube and also cannot translocate inside nanotube

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