University of Central Florida

NanoScience Technology Center
Advanced Materials Processing & Analysis Center

GRADUATE RESEARCH SEMINAR SERIES

Friday
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12:15 PM

Research Pavilion
NSTC
Conference Room 475

Pizza and drinks will be provided

Extended Simulations of the DNA Force-Extension Curve

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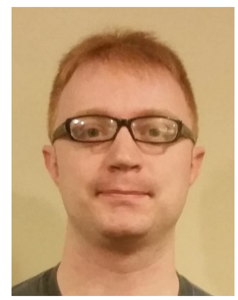
Dr. Alexander Balaeff's Group



Many processes involving nucleic acid molecules, such as packing inside the chromatin, and interaction with transcription factor and polymerase proteins, lead to structural changes of the nucleic acids under applied strain. To this end, the elastic behavior of these macromolecules is of significant interest to the scientific community. Experimental force-extension curves have been obtained for both single-stranded and double-stranded DNA. In the case of double-stranded DNA, the curves feature a prominent force plateau which indicates a phase change from B-DNA to another DNA structure. Two prevalent theories have been established in order to account for this transition. The first theory claims that the phase change is a transition from B-DNA to a disordered, or so called melted, state of DNA. The second theory claims the transition is between B-DNA and a different DNA structure: either the unwound S-DNA or the zip-DNA, in which the nucleobases from the opposite strands are interdigitating with each other.

To elucidate the nature of the DNA structural transition, we have run several extended molecular dynamics simulations at multiple points along the force-extension curve of a double-stranded DNA and measured the elastic force required to stabilize the DNA at each extension. The calculated force-extension curve qualitatively reproduces the experimental one. The analysis of the DNA conformational ensemble at each extension shows that the phase transition plateau of the force-extension curve likely results from B-DNA melting, whereas the earlier-predicted zip-DNA self-assembles gradually from the melted DNA as the DNA extends past the plateau. An extensive analysis of the DNA conformational ensemble in terms of base configuration, backbone configuration, solvent interaction energy, etc., is conducted in order to elucidate the physical origin of DNA elasticity and the main interactions responsible for the shape of the force-extension curve .