



"Soft-Matter Seminar"

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DNA: Self assembled nanostructures and complexation with hyper branched polymer

In the first part of the talk I will discuss simulation methodologies to study various DNA based nanostructures. I report MD simulation results on cross-over DNA molecules to obtain a comprehensive understanding of relationship between structure, topology, and stability of various Paranemic crossover (PX/JX) DNA molecules. The paranemic crossover (PX) DNA molecules and their topoisomers, recently synthesized by the Seeman group at New York University, are important components for novel nanomechanical devices and for constructing periodic arrays that could be useful in other nanoscale applications. In the second part of the talk I discuss the structure and dynamics of the complexation between DNA and dendrimer through atomistic molecular dynamics (MD) simulations, accompanied by free energy calculations and inherent structure determination. Complexation shows surprisingly strong sensitivity to the ssDNA sequence which is found to arise from a competition between enthalpic versus entropic rigidity of ssDNA.

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Raum PH 3344

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