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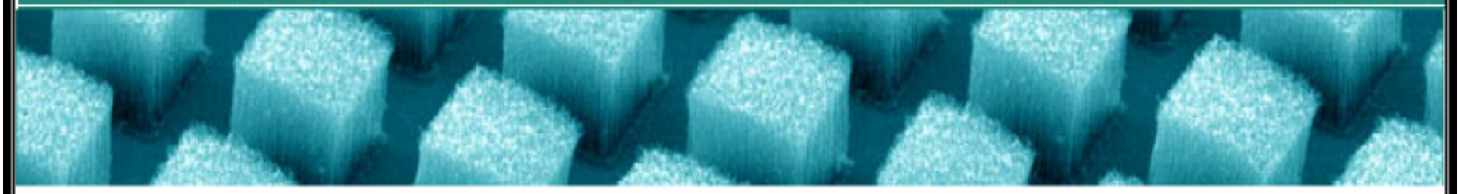

ZE SHI DISSERTATION DEFENSE
NanoEngineering Ph.D. Candidate
Arya Research Group

"Molecular-Scale Simulations of Dynamic DNA Nanostructures"

PI: Dr. Gaurav Arya

Friday, September 14, 2018
9:00a.m.
Fung Auditorium

Abstract:

Structural DNA nanotechnology, the assembly of rigid 3D structures of complex yet precise geometries, has recently been used to design dynamic, mechanically-compliant nanostructures with tunable equilibrium conformations and conformational distributions. Additional modification of such dynamic nanostructures to engineer stimuli-responsive conformational changes should further widen the possible applications of DNA nanotechnology. To provide theoretical insight and guidance on the design of dynamic DNA nanostructures, the present dissertation proposes a plan to build design tools based on coarse-grained molecular models and simulations to provide insights into the mechanical properties of dynamic DNA nanostructures, their underlying free energy landscape, and their ion-concentration-responsive behavior. In the first part of this dissertation, coarse-grained molecular dynamics simulations are used to provide insights into the conformational dynamics of a set of mechanically compliant DNA nanostructures, DNA origami hinges. An approach is also proposed for rapidly predicting equilibrium hinge angles from individual force-deformation behaviors of their single- and double-stranded DNA components. In the second part, molecular basis for the mechanism of salt-actuation of such DNA hinges is provided by computing their free energy landscape with respect to the hinge angle using a novel methodology. A simple analytical statistical-mechanical model is also introduced to model the actuation response curves obtained experimentally. This work provides some of the first molecular-scale insights into the conformational dynamics and ion-activated actuation of mechanically compliant DNA nanostructures, which should help guide the design and optimization of new nanodevices.