PHYSICS COLLOQUIUM:
Modeling and Simulation of Microtubule Polymerization and Depolymerization

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Date:
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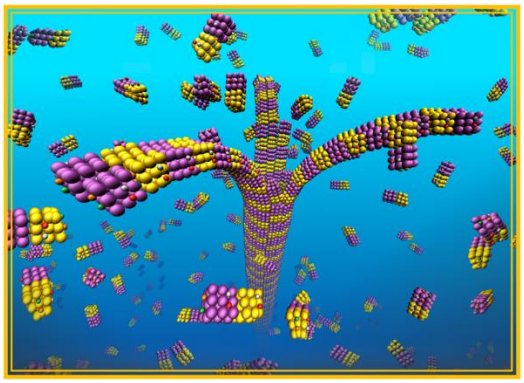
Time:
10:30 AM – 11:50 AM

Location:
GRANITE PASS 135

Abstract:

Understanding the complex self-assembly of biomacromolecules is a major outstanding question. Microtubules are one example of a biopolymer that possesses characteristics quite distinct from standard synthetic polymers that are derived from their hierarchical structure. Microtubules are stiff biopolymers that self-assemble via the addition of GTP-tubulin, but hydrolysis of GTP- to GDP-tubulin within the tubules destabilizes them toward catastrophically fast depolymerization. The molecular mechanisms and features of the individual tubulin proteins that drive such behavior are still not well-understood. To understand the fundamental features of the monomers that yield the behavior of microtubules, we have studied a minimal monomer model that self-assembles into a tubule geometry. Using molecular dynamics simulations of whole microtubules built from a coarse-grained model of tubulin, we demonstrate how conformational shape changes (i.e., deformations) in subunits that frustrate tubulin–tubulin binding within microtubules drives depolymerization of tubules via unpeeling "ram's horns" consistent with experiments. Finally, we show how catastrophic depolymerization can be interrupted by small regions of the microtubule containing undeformed dimers, corresponding to incomplete lattice hydrolysis. The results demonstrate a mechanism by which microtubule rescue can occur.



About the Speaker:

Mark J. Stevens has been on the Staff at Sandia National Laboratories since 1995. He has a BS in Physics and a BA in Mathematics from the University of Cincinnati. He received his Ph. D in physics from Johns Hopkins University in 1991. At Sandia, he started in 1995 working on the LAMMPS molecular dynamics code for parallel computers. Dr. Stevens is well known in the field of charged polymers for his groundbreaking simulations and has given many invited talks on the subject. His work has included topics such as bio membranes, polymer adhesives, colloids, dipolar fluids, lubrication and self-assembled monolayers.

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