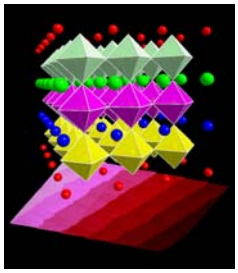
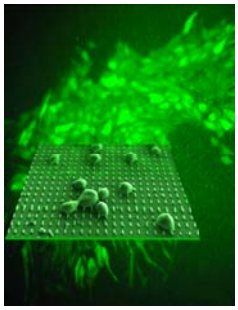
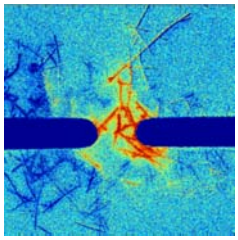
CNMS DISCOVERY SEMINAR SERIES

Monday, April 6, 2009
11:00 am
Iran Thomas Auditorium, 8600







"Atomistic and coarse-grained molecular dynamics simulations of polymers and lipids"

Ronald G. Larson
Department of Chemical Engineering, University of Michigan

Abstract:
Increasing computer speed and advanced simulation methods are now making possible to use molecular dynamics simulations to explore the dynamics of dense assemblies of large molecules. Here we use such methods to test directly the underlying assumptions of the standard "tube model" of polymer dynamics, and to estimate from molecular averages some of the parameters of the tube model such as the distribution of tube lengths, the average diameter of the tube, and the mobility of the branch point in a simple "star" branched polymer. From these developments, it is becoming possible to make a priori predictions of the rheological properties of advanced metallocene polymers, with controlled long-chain branching for optimal processing properties. We also explore the dynamics of hole formation in biological membranes produced by cationic dendrimers or aggregated antimicrobial peptides, which are important to the processes of targeted cell lysis for antimicrobial action and for drug delivery.

Hosts: Mike Kilbey, kilbeysmii@ornl.gov, 865.574.8348
Linda Horton, hortonll@ornl.gov, 865.574.5081

Center for Nanophase Materials Sciences