



DEPARTMENT OF  
MECHANICAL ENGINEERING

## The Sidney E. Fuchs Seminar Series

4:20-5:10pm, Friday, September 13, 2013  
Frank H. Walk Design Presentation Room



### Molecular Dynamics Simulation Studies of Interfacial Phenomena in Biomolecular Systems

by **Dorel Moldovan\***

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Biomolecular systems such as cell membranes, DNA, and proteins have unique attributes that make them suitable for a large number of applications of great importance in pharmaceuticals, biosciences, biomedical, and biomolecular engineering. Much of the advancements in these applications are hindered by our limited understanding of the fundamentals of these molecules structure, interaction, and transport properties in the presence of various surfaces/interfaces and biomolecular complexes. In this seminar we will present our recent investigations, using large-scale atomistic simulations and free energy calculations, into a host of open research problems pertaining to the areas of cryopreservation, drug delivery systems, and DNA sequencing. Specifically, we will present recent molecular dynamics and umbrella sampling studies of various bio-molecular systems focused on investigation of: i) the role of various chemicals in modulation of transport properties across lipid bilayers; ii) absorption and positioning of vitamin E into lipid bilayers, and on iii) understanding interaction and translocation phenomena associated with DNA mononucleotides moving through nanochannels.

\* Dr. Dorel Moldovan received a B.S. degree in 1989 in Engineering Physics from the University of Bucharest, Romania, and a M.S. and a Ph.D. degree in Physics (Computational Condensed Matter Physics) from West Virginia University in 1996 and 1999 respectively. From June 1999 to July 2001 he was a Post-Doctoral Researcher in the Materials Science Division at Argonne National Laboratory. From August 2001 to July 2002, he held a joint Visiting Research Scientist appointment with Argonne National Laboratory, and the Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany. In August 2002, he joined the Department of Mechanical Engineering at Louisiana State University where he is currently an Associate Professor. His research interests include condensed matter and materials physics focusing on various surface and interfacial phenomena such as elastic instabilities in membranes and polymers and modeling and simulation of interfacial dynamics, coarsening and microstructure evolution and deformation in nanocrystalline materials. Using atomistic, mesoscale, and continuum level simulations his recent research focuses on the development of fundamental understanding of transport and surface and interfacial phenomena in biomolecular systems.