RESEARCH SEMINAR

Thursday, April 28, 2011

3:30 p.m. – 138 DeBartolo Hall

EXPLORING THERMAL ENERGY AND MASS TRANSPORT FROM THE MOLECULAR LEVEL

Tengfei Luo

NanoEngineering Group, Department of Mechanical Engineering
Massachusetts Institute of Technology
(Faculty Candidate in Energy Separations—Aerospace and Mechanical Engineering)

Abstract

The global rising demands on energy, fresh water and cooling of microelectronics call for new understanding and novel technologies in the field of heat and mass transfer. Molecular level studies such as molecular dynamics, lattice dynamics and first-principle quantum calculations are able to probe fundamental transport phenomena at very small spatial and temporal scales where conventional theories are being challenged. In this talk, I will discuss how molecular modelings are used to understand energy and mass transport physics and stimulate engineering innovations. First, I will discuss a first-principle lattice dynamics method of predicting phonon mean-free path dependent thermal conductivity of crystals, which provides valuable guidance on fabricating nanostructured thermoelectric materials to improve their energy conversion efficiencies. Next, I will present results on thermal transport in PDMS – the most widely used polymeric thermal interface materials (TIM) in microelectronics, and I will discuss the use of self-assembled molecules as a TIM that is hundreds of times more thermally conductive than conventional polymeric TIMs. Finally, I will present a novel Directional Solvent Extraction desalination technology and discuss how to characterize and predict directional solvent properties using molecular simulations. At the end, I will also discuss my future research directions.

Bio

Dr. Tengfei Luo is a postdoctoral associate in the NanoEngineering group in Mechanical Engineering at MIT. He received his B.S. (2005) in Energy and Power Engineering at Xi'an Jiaotong University, and Ph.D. (2009) in Mechanical Engineering at Michigan State University. His research interests include simulations of nanoscale heat transfer, thermal transport across material interfaces, first-principle characterization of phonon transport, molecular modeling of water desalination and Monte Carlo simulation of hydrogen storage.