Northeastern University
College of Engineering

Please join us for a
Special Chemical Engineering Seminar

Monday, February 3, 2014
415 Shillman Hall
11:45 a.m. – 1:00 p.m.

"Multiscale Modeling of Nanomaterials in Solution"

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ABSTRACT

During this past decade, research and development in nanotechnology has made remarkable progress and has now provided a clear indication of its great potential. Among many other potential applications, nanomaterials have been investigated as promising tools in the area of biology and medicine, such as diagnostic biosensors, drug and gene delivery, and biomedical imaging. Because accomplishing these tasks requires the ability to build up the material by manipulating atoms and molecules, a detailed molecular knowledge provided by theoretical modeling is becoming increasingly important. This talk describes modeling studies of nanomaterials to characterize their stability and functionality in solution based on the all-atom molecular dynamics (MD) simulation and statistical mechanical theory of molecular liquid which is also known as 3D-RISM theory. The MD simulation captures atomic and molecular motions based on Newton's equation of motion, while 3D-RISM theory directly yields the equilibrated density distribution of solvent (solvation structure) around the solute molecule based on the statistical mechanics. In this sense, it is considered that MD simulation (kinetics) and 3D-RISM (statics) are complementary with each other. This talk will focus particularly on the association process between carbon nanotubes and nucleobases, theoretical prediction of self-assembled nanomaterial structure, and interaction between self-assembled nanomaterial and siRNA, which were conducted as collaborative projects with experimentalists.

BIOGRAPHY: Dr. Yamazaki received his PhD degree in 2002 from the Institute of Molecular Science (IMS) and the Graduate University for Advanced Studies in Japan. His PhD work was to construct a theory to predict NMR shielding constant of molecule in solution based on the RISM-SCF theory that is the hybrid theory between quantum chemistry and RISM statistical mechanical theory of molecular liquid. After spending two years as a postdoc at IMS, he moved to Canada in 2004 to join the University of Alberta and National Institute for Nanotechnology (NINT). He was a research associate in the supramolecular nanoscale assembly group where he collaborated with many experimentalists and led all aspects of theoretical modeling research.

Refreshments will be served.