Northeastern University
College *of* Engineering

Please join us for a
Special Chemical Engineering & Bioengineering Seminar

Wednesday, April 17, 2013
108 West Village H
11:45 a.m. – 1:00 p.m.

"Water, Proteins, and Interfaces: A New Molecular Perspective"

SHEKHAR GARDE, Ph.D.
Elaine S. and Jack S. Parker Professor and Department Head
The Isermann Department of Chemical & Biological Engineering
Rensselaer Polytechnic Institute, Troy, NY

ABSTRACT

Water molecules organize themselves differently near hydrophobic, hydrophilic, and ionic solutes, and near interfaces that include a combination of these characteristics (e.g., proteins). Such structural organization of water leads to water-mediated interactions, which play an important role in many self-assembly processes in aqueous solution. What are the key features of water structure and how to characterize and quantify them has, however, been a matter of controversy. I will present a new molecular level perspective based on theory and atomistic simulations that shows that nanoscale water density fluctuations provide a robust signature of hydrophobicity or philicity of complex interfaces. New computational tools are being developed based on this idea to incorporate molecular level information about water into predictive approaches for protein-ligand interactions. Physical insights into the behavior of water at interfaces also help understand how different interfaces mediate self-assembly and aggregation phenomena in their vicinity.

BIOGRAPHY: Dr. Shekhar Garde is the Elaine and Jack Parker Chaired Professor and Head of Rensselaer's Department of Chemical and Biological Engineering. He received B. Chem. Eng. (University of Bombay, 1992) and Ph.D. (U. Delaware, 1997) degrees in Chemical Engineering. He received the prestigious Director's post-doctoral fellowship at Los Alamos National Laboratory, where he performed research from 1997 to 1999. He Joined Rensselaer as an Assistant Professor in 1999. He was promoted to Associate Professor in 2004 and to Full Professor in 2006. He was appointed Parker Chaired Professor in 2006 and as the Head of Chemical and Biological Engineering Department in 2007.

His research focuses broadly on understanding the role of water in biological structure-function, and specifically on hydration and water-mediated interactions using statistical mechanical theory and molecular modeling and simulation tools. He has published 80 peer-reviewed papers in leading scientific journals which have been cited over 4000 times. He has received several awards including the prestigious CAREER Award by the US National Science Foundation (2001), School of Engineering Research Award (2003), Rensselaer Early Career Award (2004), and most recently the 2011 Robert W. Vaughan Lecturership at California Institute of Technology. Under Garde's leadership, the Chemical Engineering department climbed in US News & World Report Rankings from 33 to 22.

Dr. Garde is also one of the leaders of the unique animation movie project called the "Molecularium", which aims to excite the next generation about the world of atoms and molecules. He has pioneered integration of large-scale molecular dynamics simulations into Disney-Pixar style animation world. He is an executive producer of the Molecularium I-MAX/3-D-IMAX movies – Molecules to the MAX, which are currently being distributed nationwide. In 2011 he was honored with the Explore~Imagine~Discover Award by the Children's Museum of Science and Technology, in the Capital District, NY.

Refreshments will be served.