**Department of Chemical Engineering**

**Seminar Schedule**

**Predictive design of bio-inspired nanomaterials: Nanoscale modeling meets high-performance computing**

Trung D. Nguyen

Research Associate; Northwestern University

**Abstract**

Nanomaterials and devices that resemble biological matter in their ability to reconfigure and adapt on demand have captured increasingly growing interest in a wide range of applications including, but not limited to, biological catalysis, drug delivery, bio-sensing and energy storage and conversion. Bottom-up approaches like self- and directed-assembly are among the most promising techniques for engineering the underlying nanostructure of this exciting class of materials and devices. The fundamental challenges to these techniques are 1) to design assembling nano building blocks such as block copolymers, nanoparticles and colloids, 2) to tailor their effective interactions and 3) to find efficient assembly pathways. In this talk, I will demonstrate how computational studies supported by high performance computing have helped address these challenges. Specifically, I will discuss the design rules for several hierarchically assembled structures including terminal supraparticles, helical ribbons and columnar morphologies. I will also describe unconventional pathways to assemble bio-mimicking and reconfigurable nanostructures including interaction switching and shape shifting. Also presented are the tools and methods I have been developing to improve the efficiency of the computational studies of interest, ranging from GPU acceleration to enhanced sampling methods.

**Bio**

Dr. Trung D. Nguyen obtained his Ph.D. in Chemical Engineering at University of Michigan in 2011 under Sharon C. Glotzer. His doctoral thesis is entitled "Computer-aided design of nanostructures from self- and directed-assembly of soft matter building blocks". During 2011-2014, he served as a postdoctoral research associate at the Oak Ridge National Laboratory, where he developed massively parallel Molecular Dynamics codes for the Titan supercomputer and performed large-scale computational studies on various interfacial systems. He worked at Vietnam Academy of Science and Technology as an independent investigator during 2014-2016 before joining Monica Olvera de la Cruz's group at Northwestern University as a research associate in 2016. His research focuses on addressing exciting problems in soft matter physics with high-performance computing. His work has been recognized by the Vietnam Education Foundation Fellow Association Science Award 2012 and the MRS Communications Lecture Award 2015.

**Seminar**

**Friday, December, 8**

**10:30 am**

**Experimental Science Building 120**