UC San Diego
JACOBS SCHOOL OF ENGINEERING
NanoEngineering

UC SAN DIEGO NANOENGINEERING SEMINAR

Thursday, February 1st, 2018 11:00am – 12:00pm
Faculty Recruitment Seminar Presentation
ASML Conference Center (SME 248)

"Predictive Design of Bio-Inspired Nanomaterials: Nanoscale Modeling Meets High-Performance Computing"

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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 such as 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 describe unconventional approaches for assembling bio-mimicking and reconfigurable nanostructures such as 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.

Biosketch: Dr. Trung D. Nguyen obtained his Ph.D. in Chemical Engineering at the University of Michigan, Ann Arbor, 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 2011-14, he served as a postdoctoral research associate at the Oak Ridge National Laboratory, where he investigated interfacial effects and phase transitions in confined systems using large-scale simulations and developed massively parallel Molecular Dynamics codes for the Titan supercomputer. In 2014-16, he worked at the Vietnam Academy of Science and Technology as an independent investigator. As of 2016, he has joined Monica Olvera de la Cruz's group at Northwestern University as a research associate. His work has been recognized by the Vietnam Education Foundation Fellow Association Science Award (2012) and the MRS Communications Lecture Award (2015).