

Mechanical & Materials Engineering Pierson Graduate Seminar

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Materials and Nanoscience

Efficient Energy Transport and Storage in Functional Materials and Structures: Predictive Multi-Scale Materials Simulation and Manufacturing Process Design

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Nanomaterials, such as carbon nanotubes and graphene, and biomaterials, such as proteins and other biopolymers, are promising building blocks for smart functional materials. Being “Smart” towards external stimuli such as stress, chemical reactions, pH, temperature, and electric field, they are ideal platforms for controllable transports of energy carriers (phonons and electrons). Specifically, carbon nanomaterials exhibit ultrahigh intrinsic thermal and electronic conductance, while proteins exhibit very versatile self-assembly patterns. To scale-up materials manufacturing in functional forms, liquid-phase self-assembly, flow-processing, and heat-treatment techniques are being developed, resulting in nanofluids and nanocomposites with hierarchical structures and extensive interfaces for energy transport. To model these complex materials and structures, predictive multi-scale materials simulation is becoming a paradigm-shifting tool for *in silico* design, in response to the recent “Materials Genome Initiative”.

In this presentation, I will first introduce my computational work on structural characterizations of carbon nanomaterials in the liquid-phase to understand how they self-assemble and interact with water, which dictates their overall quality. Second, I will present my recent study on the intrinsic thermal transport in functionalized graphene and its interfacial thermal resistance with the surrounding liquid phase. This explores the potential of phonon engineering through controlled surface chemistry, and can lead to optimized performance of nanomaterials in solar thermal and heat management systems. Third, I will discuss my on-going work on the meso-scale modeling of bio-inspired flow-assembly process of biopolymers, with the potential for scalable manufacturing of superconductive fibers and composites for phonon or electron transport. Finally, I will briefly discuss my future plan to design novel battery and supercapacitor electrodes built from functionalized nanocarbon scaffolds for high performance electrochemical energy storage.

BIO

Dr. Shangchao Lin is currently a postdoctoral associate at the Laboratory of Atomistic and Molecular Mechanics (LAMM) in the Department of Civil and Environmental Engineering at Massachusetts Institute of Technology (MIT). He obtained his B.S. degree *summa cum laude* in Mechanical Engineering in 2006 from the joint program of Shanghai Jiao Tong University and the University of Michigan at Ann Arbor. He obtained his S.M. and Ph.D. degrees also in Mechanical Engineering in 2008 and 2012, respectively, both from MIT. During his graduate study, he was affiliated with the Department of Chemical Engineering at MIT and the MIT Center for Materials Science and Engineering. His research interest involves multi-scale, multi-physical simulations and computational designs of smart functional materials, using nanomaterials and biomaterials as novel building blocks with atomistic/molecular details. His future research will target integrations of fundamental principles of mechanical/chemical engineering and materials science towards exciting energy, health, and environmental applications.

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