INDUSTRIAL & SYSTEMS ENGINEERING
UNIVERSITY of WASHINGTON

MECHANICAL ENGINEERING
UNIVERSITY of WASHINGTON

ME/ISE SEMINAR: Yun Liu, Ph.D.

From Surface Chemistry to Photophysics: Understanding and Designing Materials through Atomistic Modeling and Simulations

Thursday, February 18, 12:30 PM | MEB 248

Over the past decade, challenges in energy availability and sustainability have emerged as serious global issues, which call for innovative materials research in the area of clean energy and advanced manufacturing. With atomistic modeling and simulations, we have a unique opportunity to tackle this issue through accelerated materials design using the fundamental laws of chemistry and physics. However, the dilemma between the need and the ability to model phenomena at realistic time scale and length scale often makes it challenging to utilize atomistic simulations to address real-life problems.

In this talk, I will discuss approaches to bringing together atomistic simulation methods at different scales to form solutions for engineering problems, with three examples from my research. First, I will present our discovery of the interface chemistry that governs time-dependent static friction in silica, made through multi-scale simulations. In the second example, I will demonstrate the power of high-throughput ab initio materials design with the discovery of new solar energy materials that outperform the current best candidates. Finally, I will discuss how integrating high throughput atomistic simulations with data mining enables us to develop characterization techniques that can provide molecular-level structural information of organic matter from microscopic optical measurements.

Dr. Yun Liu received his B.S. in Physics (2005) from Peking University in China and his Ph.D. in Materials Science (2012) from the University of Wisconsin - Madison. He has since been working at the Massachusetts Institute of Technology as a postdoctoral researcher in the Department of Materials Science and Engineering.

Dr. Liu's main research interests lie in energy-related fields including energy and clean energy manufacturing, with a focus on utilizing atomistic simulation methods to understand and design materials. He also works in the area of nanomechanics, interface chemistry, and seismic materials. His research makes use of multi-scale and high-throughput atomistic simulations to study contact mechanics, solar energy conversion, and energy resource exploration. The outcome of his research has led to the discovery of new interface reaction mechanisms, high performance solar energy materials, and the development of cloud-computing-based reservoir characterization techniques.