Presenting: Yao Fu, Research Associate
University of Colorado Boulder

“First-principles Based Multiscale Multiphysics Approaches for Integrated Computational Materials Engineering”

Date: Friday, February 5, 2016
Time: 3:00 - 4:00
Place: 755 Baldwin Hall

ABSTRACT

Advanced materials play key roles in the technological developments in many disciplines such as aerospace engineering, bioengineering, mechanical engineering and more. In order to reduce the cycle from design to deployment of advanced materials, integrated computational materials engineering (ICME) seeks to build a new paradigm that links design and manufacturing via materials models at multiple length scales in a seamless and integrated computational environment. In this seminar, the importance of the first-principles based multiscale/multiphysics framework to realize the ICME paradigm will be demonstrated. By providing a deeper understanding of the underlying physics of the materials and systems at various length scales, a physics-based computational predictive model would allow us to interpret and control complex materials and system behaviors. In particular, full atomistic and coarse-grained molecular dynamics simulation will be employed to investigate the microscopic structure and thermomechanical properties of polyethylene polymer and epoxy resin systems. An atomistic-continuum bridging method will be demonstrated to link the discrete nanoscale description to the continuum description in both the hierarchical and concurrent multiscale framework. Finally, the application of phase field modeling to the additive manufacturing process will be presented, and the future research directions to advance the ICME paradigm through the multiscale computational approaches will be discussed.

BIOGRAPHICAL SKETCH

Dr. Fu received her Master’s degree in materials science and engineering from the Institute of Metal Research, Chinese Academy of Sciences in 2009, and PhD degree in mechanical engineering from University of Pittsburgh in 2013. She conducted her postdoctoral studies at University of South Carolina and University of Colorado at Boulder. Dr. Fu’s research interests lie in the area of computationally guided innovative materials design and manufacturing as well as atomistic-continuum multiscale simulation to realize the integrated computational materials engineering paradigm. Her work has been published in more than 20 peer-reviewed journals and conference proceedings.