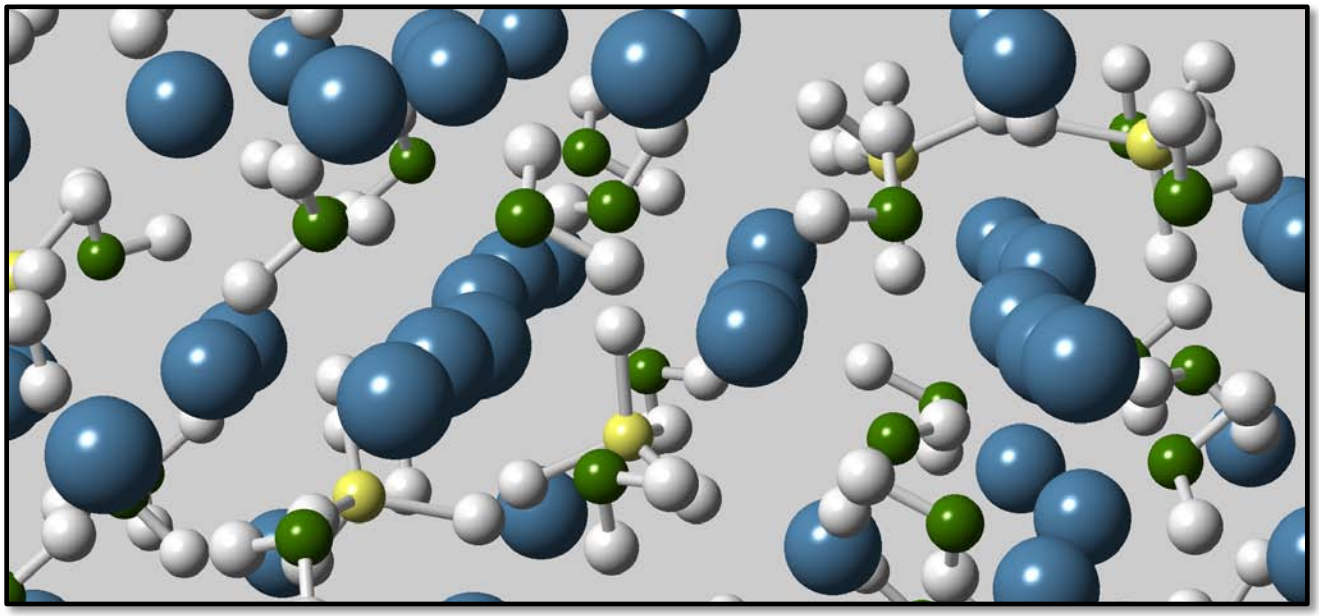

Fall 2014 Special Topics Course

Atomistic Computer Modeling of Materials

MECHENG 499/599-001, Monday and Wednesday 1:30 – 3:00PM, EWRE 185

Computational hardware and algorithms have evolved to the point where simulation can strongly complement traditional, experiment-based approaches to materials research and development. This course covers the core methods used to simulate matter at the atomic scale, and offers hands-on experience with a number of research-caliber simulation codes on multi-processor clusters. The course provides a *broad-based* and *practical* introduction to atomistic methods, and is meant to serve as a launching-point for students looking to begin independent research in this field. A variety of applications of these methods are highlighted, ranging from the mechanical properties of solids to the discovery of new materials for energy storage.

Topics:

1. Structure of matter and Inter-atomic potentials
2. High-performance computing
3. Molecular dynamics
4. Monte Carlo methods
5. Electronic structure methods: Hartree-Fock & Density Functional Theory
6. Transition state theory
7. Accelerated dynamics and multi-scale modeling

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