Computational Materials Science and Engineering
MSE 8803-C; TuTh 12:00-1:15pm, Room 299 Love
Instructors:  Prof. Rampi Ramprasad (Love 366; ramprasad@gatech.edu)
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Objectives: This course aims to provide a broad understanding of a spectrum of modern state-of-the-art computational methods used in materials science and engineering. Lectures, case studies, demonstrations and hands-on lab exercises are planned to provide theoretical depth and a practical perspective on the role of modern computational methods in revealing process-structure-property relationships and in aiding the design/discovery of new materials.


Grade: Homework (20%), 3 Midterm Exams (20% each), Final Project (20%)

Tentative Midterm Exam Dates: 9/17, 10/24, 11/21; Final Project Presentations: 12/3 or 12/12

Syllabus

Part I: Atomistic Methods

1. Why Materials Modeling?
2. Quantum Mechanics & Density Functional Theory (DFT)
3. DFT in practice
4. Classical Interatomic Potentials
5. Molecular Dynamics & Monte Carlo Simulations

Part II: Meso-scale & Macro-scale Methods

1. The United Atom Method and Coarse Graining
2. Dissipative Particle Dynamics and Mesodyn Method
3. Finite Element Methods
4. Computational Thermodynamics

Part III: Data-driven Methods: Informatics & Machine Learning

1. What is machine learning?
2. Machine learning components: data, fingerprinting, learning algorithms
3. Machine Learning in materials science
4. Other advanced methods and materials design

Part IV: Other Topics

1. Multiscale Modeling
2. Materials by Design