# 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)
Prof. Seung Soon Jang (Love 351; seungsoon.jang@gatech.edu)

**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.

**Suggested Textbooks**: (1) Ellad B. Tadmor and Ronald E. Miller: Modeling Materials: Continuum, Atomistic and Multiscale Techniques; (2) Richard Lesar: Introduction to Computational Materials Science; (3) Alexander Forrester, Andras Sobester, Andy Keane: Engineering Design via Surrogate Modelling: A Practical Guide

**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