Atomistic-Molecular Modeling and Simulation for Materials Science & Engineering MSE 8803M

Class Schedule: Tuesday and Thursday 3:30 pm – 4:45 pm
Classroom: Love 299
Mode: In-Person Mode

Syllabus

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Goal

The goal of MSE 8803M is to provide fundamental principles and practical hands-on tools of modern computational materials science, especially atomistic and molecular modeling and simulation methods based on statistical mechanics in order to achieve understanding and predictability of the structures and properties of materials systems.

Class Description

This course will be in an asynchronous remote mode. Most of the classes will be online, and the class videos will be posted in Canvas for students who can review the class contents whenever they want. The review sessions will be performed in an online format on scheduled dates. The review sessions will also be recorded and posted in Canvas. All assignments, homework, and exams will be assigned and submitted digitally. This course will have open-book exams. Each exam will be proctored via digital tools. For this, each student needs a computer with webcam, microphone, and reliable Internet connection.

Topics be covered in the lectures include:
Force Fields, Statistical Mechanics, Molecular Mechanics, Molecular Dynamics, Brownian Dynamics Simulations, Monte Carlo Simulation, Coarse-Grained Simulation, Force Field Development, and Analyses

Grading Policy

Homework 50 %
Project Report 50 % (Topic will be announced.)

Course Outline

0. Brief Review of Quantum Mechanical Methods
0.1 History of Quantum Theory, Duality, Atoms
0.2 Wave
0.3 Hartree-Fock Theory
0.4 Density Functional Theory

1. Atomistic-Molecular Interactions and Force Fields
1.1 Bonded Interactions
1.2 Non-Bonded Interactions

2. Basics of Statistical Mechanics
Temperature and Pressure, Ensembles, Boltzmann Distribution, Partition Function and State Functions, Phase Space, Time Average, Ensemble Average, and Ergodicity

3. Molecular Mechanics (MM) and Molecular Dynamics (MD) Simulation
3.1 Molecular Mechanics Simulation – Geometry Minimization
Steepest Descent, Conjugate Gradient, Newton-Raphson
3.2 Molecular Dynamics Simulation
Time evolution of Atoms – Newton's Equation of Motion, Periodic Boundary Condition, Neighbor List, Temperature Control, Pressure Control

4. Stochastic
4.1 Brownian Dynamics Simulation
4.2 Monte Carlo Simulation

5. Coarse-Grained Simulation

6. Force Field Development

7. Applications