ENMA 400 & ENMA 600 Fall 2020

ENMA 400 Introduction to Atomistic Modeling in Materials
ENMA 600 Advanced Atomistic Modeling in Materials

Instructor: Dr. Yifei Mo, 1137 Engineering Lab bldg 089, yfmo@umd.edu
Lecture Time/Room: Tuesday & Thursday 9:30-10:45 (online through ZOOM)
Lab Time/Room: The same time of the lecture (online through ZOOM)
Office Hours: TBD

Pre-requisite:

- ENMA 300: Introduction to Materials Engineering, or equivalent
- MATH 206: Introduction to MATLAB, or equivalent
- ENMA 460: Physics of Solid Materials, or Solid State Physics or equivalent
- Knowledge in Thermodynamics (ENMA 461), Physical Chemistry (CHEM481) or equivalent
- Basic knowledge in Quantum Mechanics (preferred but not required)
- Basic knowledge in Statistical Mechanics (preferred but not required)

Course Description: This is an introductory course aiming for junior/senior undergraduate students and junior graduate students to study atomistic modeling and simulation techniques used in materials research. This course covers the theories, methods, and applications of atomistic modeling techniques in simulating, understanding, and predicting the properties of materials. Specific topics include:

- Molecular statics using empirical force fields
- Quantum mechanical methods including density functional theory
- Molecular dynamics simulations
- Monte Carlo modeling and kinetic Monte Carlo modeling

Requirements and Grading:

- Lectures and computer labs will be synchronous through ZOOM. A recording will be provided for asynchronous learning.
- A lot of education activities will happen on the Canvas https://myelms.umd.edu/ . Quizzes, homework, and labs will be assigned on the Canvas, and you are required to turn in all lab reports, code, reports, presentations on the Canvas website.
- **5 Computer Labs**: Hands-on experiences of using software packages to calculate basic materials properties and to solve materials science problems. Lab reports summarizing calculation results will have to be turned in.
- **4 Homework**: MATLAB programming for basic computer modeling algorithms. Code, calculation results, and a report will have to be turned in.
- **5 Quizzes**: Short online quizzes (5-10 multiple choices and questions) to help you assess and cement your learning throughout the course.
- **Final Project**: A significant research project to be completed by the end of class. You are required for a ~15-minute presentation and a short (~3-5 page) final report. The

project topic can be anything about atomistic modeling of materials. You are encouraged to conduct project related to your research, other courses, or design project.

- **Grading**
  - Labs: 30%
  - HW: 30%
  - Quizzes: 10%
  - Final Project: 30%

Books: No class textbook. The following reference books are available electronically on Canvas or Library course reserves.

- **Modeling**
  - *Understanding molecular simulation : from algorithms to applications* / Daan Frenkel, Berend Smit. (ebook available)
  - *The ABC of DFT* / Kieron Burke and friends (ebook available)
  - *Density functional theory : a practical introduction* / David S. Sholl, Janice A. Steckel (ebook available)
  - *Computer simulation of liquids* / M.P. Allen and D.J. Tildesley
  - *Molecular modelling : principles and applications* / Andrew R. Leach
- **Statistical Mechanics**
  - *Introduction to modern statistical mechanics* / David Chandler
  - *Statistical mechanics* / Donald A. McQuarrie
- **Solid State Physics**
  - *Introduction to solid state physics* / Charles Kittel
  - *Solid state physics* / Neil W. Ashcroft, N. David Mermin.
- **Computing**
  - *MATLAB documentation*
  - *LAMMPS manual:* http://lammps.sandia.gov/doc/Manual.html
  - *VASP manual:* http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html

Software:

- Scientific Software Packages:
  - MATLAB
  - VASP
  - LAMMPS
- Visualizer of Crystal Structures
  - VESTA
  - VMD
- Unix/Linux
  - Basic shell command line
  - Text Editor: nano or gedit
  - Queue systems for HPC

Honor Code: The University of Maryland, College Park has a nationally recognized Code of Academic Integrity, administered by the Student Honor Council. This Code sets standards for academic integrity at Maryland for all undergraduate and graduate students. As a student you are responsible for upholding these standards for this course. It is very important for you to be aware of the consequences of cheating, fabrication, facilitation, and plagiarism. For more information on the Code of Academic Integrity or the Student Honor Council, please visit http://www.shc.umd.edu

Attendance Policy: Due to COVID-19, the updated University attendance policy is followed. Attendance to lectures and computer labs are best for optimal learning outcome.