ENMA 400 & ENMA 600  Fall 2017

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, CHE 2136
Lab Time/Room: The same time of the lecture, EGR 0312
Office Hours: Tuesday 11:00-12:00 pm; Wednesday 2:00-3:00 pm.

Teaching Assistant: Yizhou Zhu
TA Office Hours: TBA

Pre-requisite:
- ENMA 300: Introduction to Materials and Their Applications, 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 graduate students to study atomistic modeling and simulation techniques used in materials research. This course covers the theories, methods, and applications of atomistic-scale 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 and kinetic Monte Carlo modeling

Requirements and Grading:
- Attendance is required for all lectures the laboratories. Failure to comply will result in a lowering of your grade.
- 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 and calculation results 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 as you go.
• **Final Project:** A significant research project to be completed by the end of class. You are required for a ~15min. presentation and a short (~2 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: 15%
  – Final Project: 25%

**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

• **Computing**
  – *MATLAB documentation*

**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.

To further exhibit your commitment to academic integrity, remember to sign the Honor Pledge on all examinations and assignments: "I pledge on my honor that I have not given or received any unauthorized assistance on this examination (assignment)."

Attendance Policy: Attendance to class is required. In the event that a class must be missed due to an illness, the policy in this class is as follows:

- For every medically necessary absence from class, a reasonable effort should be made to notify the instructor in advance of the class. When returning to class, students must bring a note identifying the date of and reason for the absence, and acknowledging that the information in the note is accurate.
- If a student is absent on days when quizzes, labs, or presentations are scheduled, he or she is required to notify the instructor in advance, and upon returning to class, bring documentation of the illness, signed by a health care professional.