ENMA 489A / 698A

ENMA489A - 0101: Selected Topics in Engineering Materials;
Introduction to Computational Materials Science

ENMA698A - 0101: Special Problems in Materials Science and Engineering;
Advanced Computational Materials Science

Spring 2014

Instructor: Dr. Yifei Mo, 1137 Engr Lab Bldg 089, yfmo@umd.edu
Class & Lab Time/Room: Tuesday & Thursday 9:30-10:45, EGR 0312
Office Hours: Monday 3:30-4:30 pm, Friday 3:00-4:00 pm (Tentative)

Pre-requisite:

- ENMA 300: Introduction to Materials Science or equivalent
- ENMA 460: Solid State Physics or equivalent
- Thermodynamics, Physical Chemistry or equivalent
- Basic knowledge in computer programming or MATLAB (preferred but not required)
- 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 and senior undergraduate students and beginning graduate students to study atomistic modeling and simulation techniques that are used in materials science. This course covers the theories and applications of atomistic scale modeling techniques to simulate, understand, and predict the properties of materials. Topics include:

- Molecular statics
- Quantum mechanical methods
- Molecular dynamics simulations
- Monte Carlo simulations

Requirements and Grading:

- Attendance to class is required for both the laboratories and the lecture. Failure to do so will result in a lowering of your grade.
- This course is heavily rely on Canvas https://myelms.umd.edu/ . Quizzed, homework, labs will be assigned on Canvas, and you are required to turn them in on Canvas website.
- **5 Computer Labs**: Hands on experience using research level simulation programs to study basic materials properties. Lab reports summarizing results will have to be turned in.
- **4 Homework**: Relatively simple programs in MATLAB, including an initial assignment to help you learn the language. Code and results will have to be turned in.
- **5 quizzes**: These will be short quizzes and help you assess and cement your learning as you go.
- **Final Project**: This will be a significant project with a ~15min. presentation and a short (~2 page) final report, to be completed by the end of class. You will form two-people groups and you are graded as a group. The subject can be almost any issue in atomistic modeling, including writing your own program and using existing programs.
- **Grading**
  - Labs: 30%
  - HW: 30%
  - Quizzes: 15%
  - Final Project: 25%

Books: No class textbook (in course reserves or available electronically through Canvas or the Library)

- **Modeling**
  - *Understanding molecular simulation : from algorithms to applications* / Daan Frenkel, Berend Smit. (ebook available)
  - *Computer simulation of liquids* / M.P. Allen and D.J. Tildesley
  - *Molecular modelling : principles and applications* / Andrew R. Leach (at Chemistry Library reserves desk)
  - *The ABC of DFT* / Kieron Burke and friends (ebook available)
  - *Density functional theory : a practical introduction* / David S. Sholl, Janice A. Steckel (ebook available)
- **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*

Software:

- Scientific Packages:
  - MATLAB
  - VASP
  - GULP
- 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.

Tentative Class schedule and Due dates: (subjected to changes)

Tu	1/28	Introduction to atomistic modeling	HW1 Assigned
Th	1/30	Computers, Languages, and Introduction to MATLAB	
Tu	2/4	Classical Mechanics	
Th	2/6	Molecular Statics	HW1 Due on 2/9
Tu	2/11	Lab1: Unix & HPC. Get familiar with Deepthought	HW2 assigned; Quiz 1 assigned
Th	2/13	(University Closed: Cancelled due to Snow Emergency)	Quiz 1 due on 2/16
Tu	2/18	Classical potential I - Basic pair potentials	
Th	2/20	Classical potential II - Many-body potentials	
Tu	2/25	Lab 2: Molecular Statics	Quiz 2
Th	2/27	Molecular Dynamics I - Integrating F=ma, time steps;	HW2 Due 2/25; HW3 Assigned
Tu	3/4	Molecular Dynamics II - Thermostat	
Th	3/6	Molecular Dynamics III - Simulation analysis, limitations	
Tu	3/11	Lab 3: Molecular Dynamics	Quiz3
Th	3/13	Quantum Mechanics I: Introduction	HW3 Due
Tu	3/18	Spring Break	
Th	3/20	Spring Break	
Tu	3/25	Quantum Methods II: Basic Applications	Final project assigned
Th	3/27	Quantum Methods III: Key Concepts of DFT	
Tu	4/1	Quantum Methods IV: Introduction to VASP	
Th	4/3	Lab 4: Quantum Mechanics - DFT1	Final Projects Proposal Due
Tu	4/8	Quantum Methods V: Applications and Materials Project	
Th	4/10	Lab 5: Quantum Mechanics - DFT2	Quiz4
Tu	4/15	Monte Carlo I - State space sampling, Classical momentum	HW4 Assigned
Th	4/17	Monte Carlo II - Metropolis algorithm, simulation analysis	
Tu	4/22	(MRS week) Final Project Proposal Review	Time/Date TBD
Th	4/24	(MRS week) Final Project Proposal Review	Time/Date TBD
Tu	4/29	Advanced topics: Kinetic Monte Carlo; Accelerated MD.	Quiz 5; HW4 Due
Th	5/1	Final Project Presentations (3-4)	
Tu	5/6	Final Project Presentations (3-4)	
Th	5/8	Final Project Presentations (3-4)	
Tu	5/13	Final Project Presentations (3-4)	Last day of class
Th		Final week schedule TBD	Final project Due