ASEN 6519: Molecular Simulation of Materials

Spring 2023

Class meetings: Tue/Thu 11:30 AM - 12:45 PM AERO N250
Join Zoom Meeting (Meeting ID: 958 1240 7362)

Instructor:

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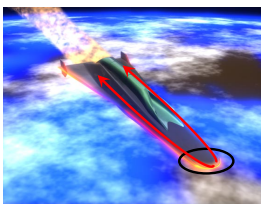
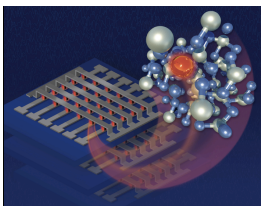
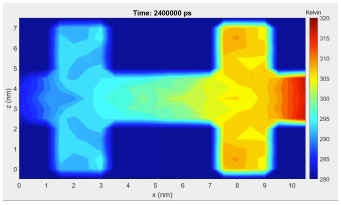
Course Description, Objective, and Outcomes:

When the relevant transformation of a material or a structure occurs over length scales on the order of atomic spacings and time scales on the order of the period of atomic vibrations, one cannot rely on continuum descriptions of materials to accurately describe the phenomena. Dynamic restructuring of materials surfaces or interfaces, oxidation of microstructures in composite materials or ceramics at high-temperatures or in highly chemically-active environments are some examples of such phenomena. The theoretical formulations can be complex and often cannot fully describe the physical mechanisms responsible for the transformations. At the same time, performing experiments can be challenging as well as expensive.

Numerical techniques offer the remarkable opportunity to predict atomic level phenomena and provide guidance to experimental studies. Molecular modeling and simulations thus emerged as an essential tool for not only predicting the materials performance in diverse environments but designing novel materials with desired functionalities and performance. Predictive modeling of materials at the atomic scale is of great interest in a broad range of technological applications, including electronic, optoelectronic, energy conversion, renewable energy harvesting, chemical-sensing, bio-medical and quantum devices.

The objective of this course is to expose students to the theory and implementation of numerical techniques for modeling behavior of materials at the atomic level. The numerical technique of focus will be classical molecular dynamics simulations. One of the main applications that will be discussed in this course is the analysis of heat conduction properties of materials. If we can control heat conduction in materials, we will be able to design leading edges of aerospace vehicles that are capable of flying at supersonic and hypersonic speeds, engineer thermoelectric materials with improved efficiency for deep space explorations and design next generation radiation-hard microelectronics based on wide and ultra-wide-band-gap semiconductors. In this course, you will

- Learn the theory behind molecular dynamics (MD) simulations.
- Write your own MD code to perform simulations.
- Critically assess published results from MD simulations for technical correctness and physical relevance.
- Analyze MD results to obtain physically measurable parameters.
- Design your class project to model materials in different environmental conditions.
- Learn to use the open-source software, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), to model atomic level phenomena accurately.

Logistics:

A. Office hours

TBD

B. Class Time

There are two 75-mins meetings per week. The time will include formal lecturing, computer demonstrations, and group work. You are responsible for all material discussed in class, whether you attended or not. Class schedule is posted on Canvas, subject to change.

C. Prerequisites

Students are expected to have taken an undergraduate thermodynamics course. Background knowledge in hamiltonian formulation of classical mechanics, statistical mechanics, and solid state physics will be helpful but is not required. Experience with computer programming is going to be helpful but extensive previous experience is not required. It is strongly recommend to work in a Linux-based platform. Students are free to program in a language of their choice, however it is advised to use Python/Matlab/Fortran for coding/scripting purposes. Some of the assignments will be based on using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software.

D. Website

Course materials are available on Canvas.

E. Reading Material

The textbook for the course will be

- *Statistical Mechanics: Theory and Molecular Simulation*, Mark E. Tuckerman, Oxford, 2010
  eBook available online through CU Boulder Libraries;
  Link: https://ebookcentral.proquest.com/lib/ucb/detail.action?docID=3053587.

The following books may be useful for reference. You will also be provided with notes and papers from the literature during the semester.

- *Computer Simulation of Liquids*, M. P. Allen and D. J. Tildesly, Oxford, 1989, ISBN 9780198556459.
- *Introduction to Modern Statistical Mechanics*, D. Chandler, Oxford, 1987, ISBN 9780195042771.

F. Grades

Homework (35%), two mid-term exams (30%), class participation (5%), and project (30%);

(a) Homework assignments: 35%

There will be six homework assignments in the course. There will be pencil and paper problems and programming assignments. Students are encouraged to work together but must submit their own work for grading. If applicable, you must indicate in your submission who you worked with. For programming assignments, documentation within the code is strongly recommended. It is necessary than your final submitted code runs without giving an error.

Homework will be due on **Fridays at 11:59 PM** and should be submitted to Canvas. Please put all files (code, text documents, scanned files) into one zip file with the naming scheme (last- name)HW(homework number).zip. For example, neogiHW4.zip. Recommended file types are: pdf, jpg, png etc for documents and figures. Homework submitted by 8 AM the day after it is due will be penalized 25%. Homework submitted by midnight of the day after it is due will be penalized 50%. Homework submitted after that time will result in a grade of zero.

(b) Case Study/Project presentations and reports: 30%

Details will be provided in class. The deadline policies will be similar to homework submission policies.

(c) Class participation for regular students: 5%

The students will be required to provide peer review for presentations, for example. More details will be provided in class.

Any grading disputes will be handled by the instructor. Any request for a grade change should be made to the instructor, in writing, **within one week after the graded work is returned**. Your entire submission will be subject to regrading. Students are advised to read and adhere to the Honor Code at the University of Colorado at Boulder.

(d) Exam dates (tentative):

- **Mid-term Exam 1:** TBD
- **Mid-term Exam 2:** TBD
- **Case Study/Final Project Presentations:** Wednesday, May 10 4:30 PM–7:00 PM or before.

Course content:

1. Introduction to molecular simulation
   (a) Model systems
   (b) Empirical potentials
   (c) Finite systems: Consideration of boundary conditions
2. Review of classical mechanics
   (a) Newton's laws of motion
   (b) Phase space: Visualizing classical motion
   (c) Hamiltonian formulation of classical mechanics
3. Introduction to classical statistical mechanics
   (a) The laws of thermodynamics
   (b) The ensemble concept: connection between the macroscopic and the microscopic worlds
   (c) Types of statistical ensembles
4. The microcanonical ensemble and introduction to molecular dynamics
   (a) Conditions for thermal equilibrium
   (b) Initialization
   (c) Equations of motion, energy calculations
   (d) Integrating the equations of motion: Finite difference methods
5. The canonical (constant-temperature) ensemble
   (a) Energy fluctuations in the canonical ensemble
   (b) Determining structure and thermodynamics in real gases and liquids
   (c) Constant-temperature molecular dynamics
6. Classical time-dependent statistical mechanics

(a) Externally driven systems and linear response theory

(b) Application of linear response theory: Transport coefficients

(c) Calculating time correlation functions from molecular dynamics

(d) The nonequilibrium molecular dynamics approach

There might be lectures on advanced topics in addition to the above content, mainly on modeling thermal properties of materials. The computer demonstrations/workshop activities will be carried on with LAMMPS.