ASEN 6519: Molecular Modeling of Materials

Spring 2026

Class meetings: Tue/Thu 11:30 AM - 12:45 PM AERO N250

Instructor:

Prof. Sanghamitra Neogi
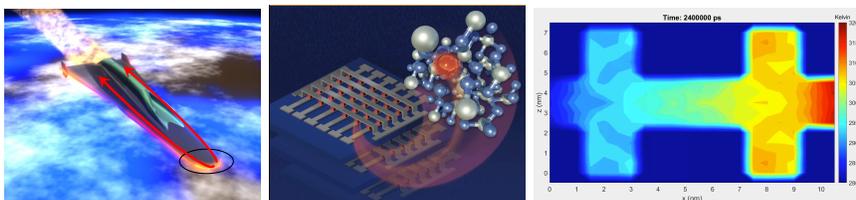*E-mail*: sanghamitra.neogi@colorado.edu

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 introduce students to the theory and implementation of numerical techniques for modeling materials at the atomic scale, with a primary focus on classical molecular dynamics simulations. A key application explored in the course is the analysis of heat conduction in materials. Control of heat transport enables faster and more energy-efficient microelectronics through advanced thermal management, high-efficiency thermoelectric materials for deep-space exploration, and aerospace vehicle leading edges capable of sustained supersonic and hypersonic flight. More broadly, atomic-scale materials control underpins radiation-hard electronic and optoelectronic technologies, where defect formation, disorder, and non-equilibrium energy dissipation govern robustness in extreme environments, as well as solid-state quantum devices, in which phonons, defects, and interfaces determine the coherence and stability of information being processed.

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 for different technological applications.

- 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

Tue/Thu 01:30 - 02:30 PM, otherwise by appointment.

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. A tentative class schedule will be posted on Canvas, subject to change. *Class will not be held on February 26, in observance of the campus Midterm Reading Day.*

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.

- *Computer Simulation of Liquids*, M. P. Allen and D. J. Tildesly, Oxford, 2017, ISBN 9780191841439 (ebook)
  Link: https://doi-org.colorado.idm.oclc.org/10.1093/oso/9780198803195.001.0001.

- *Introduction to Modern Statistical Mechanics*, D. Chandler, Oxford, 1987, ISBN 9780195042771.

F. Grades

Homework (40%), two mid-term exams (25%), class participation (5%), and project (30%);

(a) Homework assignments: 40%

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, to receive credit.

Homework will be due on **Fridays at 11:59 PM** and should be submitted to Canvas or Gradescope. 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) Project presentations and reports: 30%

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

(c) Participation: 5%

   The students will be required to provide peer review for presentations. 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:** Thursday, March 5, 2026
   - **Mid-term Exam 2:** Thursday, April 9, 2026
   - **Final Project Presentations:** Thursday, April 30 10:30 AM.–1 PM or before. We might need the entire time till 1:00 PM, please make your travel arrangements accordingly.

Tentative List of Course Topics:

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, more details will be provided in class.

Honor Code

All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the Honor Code. Violations of the Honor Code may include but are not limited to: plagiarism (including use of paper writing services or technology [such as essay bots]), cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty. Understanding the course's syllabus is a vital part of adhering to the Honor Code.

All incidents of academic misconduct will be reported to Student Conduct & Conflict Resolution: Student-Conduct@colorado.edu. Students found responsible for violating the Honor Code will be assigned resolution outcomes from Student Conduct & Conflict Resolution and will be subject to academic sanctions from the faculty member. Visit Honor Code for more information on the academic integrity policy.

Accommodation for Disabilities, Temporary Medical Conditions, and Medical Isolation

If you qualify for accommodations because of a disability, please submit your accommodation letter from Disability Services to your faculty member in a timely manner so that your needs can be addressed. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the Disability Services website. Contact Disability Services at 303-492-8671 or DSinfo@colorado.edu for further assistance. If you have a temporary medical condition, see Temporary Medical Conditions on the Disability Services website.

If you have a temporary illness, injury or required medical isolation for which you require adjustment, please contact the instructor at the earliest convenience. We do not require students to state the nature of their illness when alerting us.

Accommodation for Religious Obligations

Campus policy requires faculty to provide reasonable accommodations for students who, because of religious obligations, have conflicts with scheduled exams, assignments, or required attendance. Please communicate the need for a religious accommodation in a timely manner. In this class, you should make arrangements with the instructors at least two weeks in advance, so that appropriate accommodations can be made. See the campus policy regarding religious observances for full details.

Preferred Student Names and Pronouns

CU Boulder recognizes that students' legal information does not always align with how they identify. If you wish to have your preferred name (rather than your legal name) and/or your preferred pronouns appear on your instructors' class rosters and in Canvas, visit the Registrar's website for instructions on how to change your personal information in university systems.

Classroom Behavior

Students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in person, remote, or online. Failure to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed, religion, sexual orientation,

gender identity, gender expression, veteran status, marital status, political affiliation, or political philosophy.

Additional classroom behavior information

- Student Classroom and Course-Related Behavior Policy.

- Student Code of Conduct.

- Office of Institutional Equity and Compliance.

Sexual Misconduct, Discrimination, Harassment and/or Related Retaliation

CU Boulder is committed to fostering an inclusive and welcoming learning, working, and living environment. University policy prohibits protected-class discrimination and harassment, sexual misconduct (harassment, exploitation, and assault), intimate partner abuse (dating or domestic violence), stalking, and related retaliation by or against members of our community on- and off-campus. The Office of Institutional Equity and Compliance (OIEC) addresses these concerns, and individuals who have been subjected to misconduct can contact OIEC at 303-492-2127 or email OIEC@colorado.edu. Information about university policies, reporting options, and OIEC support resources including confidential services can be found on the OIEC website.

Please know that faculty and graduate instructors are required to inform OIEC when they are made aware of incidents related to these concerns regardless of when or where something occurred. This is to ensure the person impacted receives outreach from OIEC about resolution options and support resources. To learn more about reporting and support a variety of concerns, visit the Don't Ignore It page.

Mental Health and Wellness

The University of Colorado Boulder is committed to the well-being of all students. If you are struggling with personal stressors, mental health or substance use concerns that are impacting academic or daily life, please contact Counseling and Psychiatric Services (CAPS), located in C4C, or call (303) 492-2277, 24/7.

Acceptable Use of AI in This Class

Generative artificial intelligence tools—software that reproduces text, images, computer code, audio, video, and other content—have become widely available. Well-known examples include ChatGPT for text and DALL·E for images. This statement governs all such tools, including those released during our semester together.

Keep in mind that the goal of gen AI tools is to reproduce content that seems to have been produced by a human, not to produce accurate or reliable content; therefore, relying on a gen AI tool may result in your submission of inaccurate content. It is your responsibility—not the tool's—to assure the quality, integrity, and accuracy of work you submit in any college course.

If gen AI tool use is suspected in completing assignments for this course in ways not explicitly authorized, I will follow up with you. I may contact the Office of Student Conduct & Conflict Resolution to report suspected Honor Code violations. In addition, you must be wary of unintentional plagiarism or data fabrication. Please act with integrity, for the sake of both your personal learning and your academic record.

Other Policies Please be respectful of others during class time. This includes turning off your cell phone before class and not talking during class unless you have the floor. Details about all of the university policies can be found on the web at https://www.colorado.edu/academicaffairs/policies-customs-guidelines.