(1a) (2) (1b)
MECH 8XX*/3.0 Introduction to Computational Materials Science
This course focuses on atom-scale modelling of materials using computational methods. Covered topics include electronic density functional theory, molecular dynamics, Metropolis Monte Carlo, and transition state theory. The course will cover fundamental theoretical aspects and hands-on application of the methods. It will include a short, open-ended, end-of-semester simulation project.

Course description

This course is an elective. The intent is to provide the students with the necessary knowledge and experience to perform atomistic simulations of materials. This course will emphasize a programing-based approach to learning. The course will cover the following topics:

- **Electronic density functional theory**
- **Molecular dynamics**
- **Metropolis Monte Carlo**
- **Transition state theory**

Electronic density functional theory (DFT)
Timeframe: ~3 weeks
This will be a brief introduction to DFT. Most likely, we will cover the first few chapters of "Density Functional Theory—A Practical Introduction", by David Sholl and Janice Steckel (likely chapters 1,2,3, & 5). Themes include an introduction to DFT, setting up simple simulations of solids, understanding the main parameters (choice of X-C functional, basis set, k-points, etc.), and performing vibrational analysis. The students will familiarize themselves with the main approximations involved in DFT calculations, and how to set up and analyze the output of these simulations.

While a quantum mechanics / solid state physics / physical chemistry background is an asset, it is not a prerequisite. However, the course will emphasize that DFT simulations should be interpreted with caution, and that it may be necessary to develop such a background before running such simulations.

The students will install Quantum Espresso (a free/libre code), and run small simulations on their personal computer.

Molecular dynamics (MD)
Timeframe: ~2 weeks
This will be an introduction to MD. Most likely, we will cover chapters 1, 2, 3, 5, 6, & 8 of "Computational Materials Science—Fundamental to Applications", by Richard Lesar. We will cover interatomic interaction potentials, structural optimization algorithm, the velocity-Verlet algorithm, ensembles, thermostats, barostats, measurements, and coarse-graining.

While a statistical mechanics / solid state physics background is an asset, it is not a prerequisite. However, the course will emphasize that, similarly to DFT, MD simulations should be interpreted with caution, and that it may be necessary to develop such a background before running such

simulations.

The students will install LAMMPS (a free/libre code), and run small simulations on their personal computer.

Monte Carlo (MC)
Timeframe: ~2 weeks
Most likely, we will cover chapters 7 of "Computational Materials Science—Fundamental to Applications", by Richard Lesar. We will also cover chapters 3, 5, 7, & 8 "Computational Science—From Theory to Applications" by Frenkel, Klein, Parrinello, and Smit. We will cover ensembles, Metropolis MC, GCMC, Gibbs ensemble MC and biased sampling.

While a statistical mechanics / solid state physics background is an asset, it is not a prerequisite. However, the course will emphasize that, similarly to MD and DFT simulations should be interpreted with caution, and that it may be necessary to develop such a background before running such simulations.

Transition state theory
Timeframe: ~2 weeks
In this section, we will likely cover chapter 9 of the Lesar textbook, and chapter 6 of the Sholl textbook. In addition, we will rely on review articles in the literature about saddle-point search methods, as well as accelerated molecular dynamics. The idea is to be able to search and refine transition states, as well as use this information to perform mesoscale simulations.

Small project
Timeframe: ~3 weeks

The students will perform a 3-week individual simulation project. The theme will be decided on a case-by-case, student-by-student basis, depending on their interests and abilities.

Instruction style

Students will familiarize themselves with the content of the required reading before class. Time in the classroom will be spent reinforcing these theoretical concepts (small quizzes, discussions, mini-lectures given both by the instructors and the students, etc.). Afterwards, under the supervision of the instructor, the students will begin a computer-based assignment, which they will complete on their own time. One assignment will be due each week for the first 9 weeks. The last three weeks will be spent working on the project, with weekly in-class help/advice of the instructor.