

# CHEM 5100: Advanced Computational Modeling

## Fall 2020

### Instructor Information

*Name:* Laura de Sousa Oliveira  
*Office:* 408 Physical Sciences  
*Email:* Laura.deSousaOliveira@uwyo.edu  
*Office Hours:* TBD — Online

### Class Information

*Dates:* August 25<sup>th</sup> – December 10<sup>th</sup>, 2020  
*Time:* 2:45 – 4:00 PM (Mountain Daylight Time) · Tuesday/Thursday  
*Classroom:* N/A Online  
*Platform:* Zoom  
*Credits:* 3 credit hours

### Course Description

Computational modeling is a third pillar of science, alongside experiment and theory. This class introduces several advanced modeling techniques used in solid state chemistry and focuses on atomistic methods, such as molecular dynamics and density functional theory. The class is taught through hands-on projects in which the students use computational approaches to investigate important concepts in solid state chemistry. The aim is that in addition to learning about modeling and simulation, students will develop an understanding of how and when to use these tools effectively, and how to analyze and critically assess results. Specific topics are outlined in the schedule.

*Prerequisites:* basic programming experience.

### Student Learning Outcomes

After this course, you should be able to:

- Improve your ability to engage in critical thinking, reasoning, and communication in the field of computational modeling.
- Gain an understanding of the capabilities and limitations of computer simulations in solid state chemistry.
- Develop a matured perspective on how to approach chemistry problems through the lens of computational modeling.

More specifically, you should gain a practical understanding of:

- Molecular statics, in particular the applicability and limitations of atomic potentials.
- The anatomy of molecular dynamics simulations.

- Density functional theory (DFT) within the context of first principles approaches, and its application, among other things, to predict configurational energies and the electronic structure of molecules/materials.

## Textbooks

You are not required to purchase any book. The books below are just suggestions for your edification. Note that all of the books listed are available to you online as e-books through the University of Wyoming Library.

- Frenkel, Daan, and Berend Smit. **Understanding molecular simulation: from algorithms to applications**. Vol. 1. Elsevier, 2001.
- Ramachandran, K. I., Gopakumar Deepa, and Krishnan Namboori. **Computational chemistry and molecular modeling: principles and applications**. Springer Science & Business Media, 2008.
- Ohno, Kaoru, Keivan Esfarjani, and Yoshiyuki Kawazoe. **Computational materials science: from ab initio to Monte Carlo methods**. Springer, 2018.

## Grading

There are no exams or quizzes. Grading is based on **4 projects (10% for the first project and 20% for projects 2–4)**, and a **final project (20%)**, including a **1 page research proposal (5%)**, and an **oral presentation (5%)**. You are expected to produce an *individual* report for each project. You have ~ 3 weeks to complete each project and write the report (see tentative deadlines in the schedule below). The final project will be independent, and should relate to your research, if possible, or be on a topic of your interest if you don't have a research project yet. Note that the reports must include the code or scripts used towards the project.

If you need an extension for any reason, contact the instructor in a timely fashion, as permitted by the need. There is no guarantee that you will receive an extension on any assignment, so plan accordingly. Finally, you are welcome (encouraged, even) to work with others *provided you can do so safely*. You are, however, expected to submit your own work.

## Class Methodology & Tentative Schedule

An important aspect of the course set-up is to learn the methods and reinforce concepts by applying them. The classes will therefore be a combination of lectures and hands-on computational labs, where you can work collectively and ask questions to the instructor. You are expected to make progress in the assigned projects during the *hands-on* classes, and you will be asked to share your screen on occasion. This is an online synchronous course, meaning you are expected to attend class at the time it is offered.

*Tentative* schedule and list of topics for the course:

### - Week of 08/25:

*Lecture*: Overview and history of computation and modeling; good computational practices.

*Hands-on*: How to use terminal. You will be given access to the local HPC resources, where you will be expected to perform all computational tasks. You can do this from anywhere, all you need

is a computer with a "terminal" application and an internet connection.

**- Weeks of 09/01 and 09/08:**

*Lecture/Hands-on:* The Ising model in the context of Monte Carlo simulations.  
*Due:* Project 1 report due on 09/15 (Tuesday), worth 10% of your final grade.

**- Weeks of 09/15, 09/22 and 09/29:**

*Lecture/Hands-on:* Molecular statics: e.g., fundamentals of empirical atomic potentials, energy minimization, the dynamical matrix.  
*Due:* Project 2 report due 10/06 (Tuesday), worth 20% of your final grade.

**- Weeks of 10/06, 10/13, and 10/20:**

*Lecture/Hands-on:* Molecular dynamics: e.g., Verlet and other integration algorithms, thermodynamic ensembles, thermostats, the velocity autocorrelation.  
*Due:* Project 3 report due 10/27 (Tuesday), worth 20% of your final grade.

**- Weeks of 10/27, 11/03, and 11/10:**

*Lecture/Hands-on:* Density functional theory within the context of *ab-initio* approaches: e.g., Kohn-Sham formalism, basis sets, exchange correlational functionals, configurational energies, electronic structure of molecules/materials.  
*Due:* 1 page proposal (for final project), worth 5% of your grade, due 11/10 (Thursday). Project 4 report, worth 20% of your final grade, due 11/17 (Tuesday).

**- Week of 11/17:**

*Lecture:* Discussion of final project topics & approaches.  
*Hands-on:* Begin working on final project.

**- Weeks of 11/24 and 12/01:**

*Lecture:* Overview of other modeling approaches: e.g., finite element, multi-scale modeling, tight-binding, time-dependent DFT.  
*Hands-on:* Work on your final project. You will be expected to show progress and be able to discuss the project in class.  
*Due:* Final project, worth 20% of your grade, due 12/03 (Thursday).

**- Week of 12/08:**

Oral presentations (worth 5% of your grade).

## **Disability Support**

The University of Wyoming is committed to providing equitable access to learning opportunities for all students. If you have a disability, including but not limited to physical, learning, sensory or psychological disabilities, and would like to request accommodations in this course due to your disability, please register with and provide documentation of your disability as soon as possible to Disability Support Services (DSS), Room 128 Knight Hall. You may also contact DSS at (307) 766-3073 or [udss@uwyo.edu](mailto:udss@uwyo.edu). It is in the student's best interest to request accommodations within the first week of classes, understanding that accommodations are not retroactive. Visit the DSS website for more information at: [www.uwyo.edu/udss](http://www.uwyo.edu/udss).

## **Classroom Statement on Diversity**

The University of Wyoming values an educational environment that is diverse, equitable, and inclusive. The diversity that students and faculty bring to class, including age, country of origin, culture, disability, economic class, ethnicity, gender identity, immigration status, linguistic, political affiliation, race, religion, sexual orientation, veteran status, worldview, and other social and cultural diversity is valued, respected, and considered a resource for learning.

## **Academic Dishonesty Policies**

Academic dishonesty will not be tolerated in this class. Cases of academic dishonesty will be treated in accordance with UW Regulation 2-114. The penalties for academic dishonesty can include, at my discretion, an “F” on an exam, an “F” on the class component exercise, and/or an “F” in the entire course. Academic dishonesty means anything that represents someone else’s ideas as your own without attribution. It is intellectual theft – stealing - and includes (but is not limited to) unapproved assistance on examinations, plagiarism (use of any amount of another person’s writings, blog posts, publications, and other materials without attributing that material to that person with citations), or fabrication of referenced information. Facilitation of another person’s academic dishonesty is also considered academic dishonesty and will be treated identically.

## **Classroom Behavior Policy**

At all times, treat your presence in the classroom and your enrollment in this course as you would a job. Act professionally, arrive on time, pay attention, complete your work in a timely and professional manner, and treat all deadlines seriously. You will be respectful towards you classmates and instructor. Spirited debate and disagreement are to be expected in any classroom and all views will be heard fully, but at all times we will behave civilly and with respect towards one another. Personal attacks, offensive language, name-calling, and dismissive gestures are not warranted in a learning atmosphere. As the instructor, I have the right to dismiss you from the classroom, study sessions, electronic forums, and other areas where disruptive behavior occurs. Electronic devices such as mobile phones should be left at home or turned off.

## **Duty to Report**

UW faculty are committed to supporting students and upholding the University’s non-discrimination policy. Under Title IX, discrimination based upon sex and gender is prohibited. If you experience an incident of sex- or gender-based discrimination, we encourage you to report it. While you may talk to a faculty member, understand that as a "Responsible Employee" of the University, the faculty member **MUST** report information you share about the incident to the university’s Title IX Coordinator (you may choose whether you or anyone involved is identified by name). If you would like to speak with someone who may be able to afford you privacy or confidentiality, there are people who can meet with you. Faculty can help direct you or you may find info about UW policy and resources at <http://www.uwyo.edu/reportit>.

## COVID-19 Policies

During this pandemic, you must abide by all UW policies and public health rules put forward by the City of Laramie (or by Natrona County if at UW-Casper), the University of Wyoming and the State of Wyoming to promote the health and well-being of fellow students and your own personal self-care. Please review the current policy: <https://www.uwyo.edu/alerts/campus-return>.

As with other disruptive behaviors, the instructor has the right to dismiss you from the classroom (Zoom and physical), or other class activities if you fail to abide by these COVID-19 policies. These behaviors will be referred to the Dean of Students Office using the UWYO Cares Reporting Form for Student Code of Conduct processes.

Syllabus changes:

You will be alerted to any possible course format changes in response to UW decisions about community safety during the semester.

Online course expectations:

As with all UW coursework, this course will be educational and useful to you. The instructor commits to responding to questions, concerns, and feedback in a timely manner.

Your responsibilities:

- Give and receive feedback from the instructor and your classmates respectfully and constructively in all interactions. This includes in Zoom chats, on WyoCourses boards, and within physical classroom spaces.
- Actively engage in civil discourse in a respectful manner. Use professional language in all course related forums.
- Communicate professionally. Whenever you send class-related email or messages, please include a clear, specific subject line and use the body of the email or message to explain the purpose for the email and any attached materials. Conduct yourself professionally.
- Meet assignment deadlines. We expect that you're interacting with course material multiple times during the week.
- Ask for help when you need it. For academic assistance for this course please contact the instructor for available resources.
- Please let us know if you notice another student who needs help in the University's (anonymous) WyoCares referral option: <https://www.uwyo.edu/dos/students-concern>

## Zoom Protocol

Lectures and demos will be recorded, not including video with the exception of shared screens. Cameras should be on at all times except during breaks.