CHBE 451 2024W

Course Syllabus

WELCOME STATEMENT

I would like to acknowledge that UBC's Vancouver Point Grey campus is situated on the traditional, ancestral, unceded territory of the xʷməθkʷəy̓əm (Musqueam) people. To find out which land(s) you are on: https://native-land.ca/

Links to an external site.. For PD on how to develop virtual land acknowledgements with respect and sincerity:

https://wpl.ubc.ca/browse/professional-development/courses/wpl-pd-rsr

Course Description

In this course, we will build the fundamental concepts of thermodynamics from both classical and statistical mechanics perspectives. Fundamental equations of thermodynamics and various other laws will be derived using statistical thermodynamic theory, providing molecular interpretation of basic concepts such as energy and entropy, with an emphasis on the relationship between bulk (macroscopic) behaviour and molecular interactions. Simple models of gases, liquids and solids will be reviewed. These methods will be applied to the analysis of various systems and processes using molecular simulations. Current research questions in engineering will be addressed using simplified physical models.

Instructor

Simcha Srebnik, simcha.srebnik@ubc.ca (she/her).

Office: CHBE 419.

The best way to contact me is via email and office hours. I will do my best to answer the same day (if contacted before 6 pm). I tend to be less available on weekends and holidays.

Lectures

M 10:00-11:20 am   Room: SWNG 309

W 10:00-11:20 am   Room: SWNG 309

Office Hours

~~**M** 11:30am-12:30pm Room: CHBE 419~~

M 1-2 pm Room: CHBE 419

Class Zoom Room

The following class Zoom room will be used for online meetings:

Zoom Room ID: 664 0921 3646 Passcode: 804649

https://ubc.zoom.us/j/66409213646?pwd=cjJienM2RXk0QTBtb3o5RllPKzc2Zz09

Links to an external site.

Required textbook

- *Thermodynamics and Statistical Mechanics - An Integrated Approach*
- Links to an external site. by M. Scott Shell, Cambridge Press, 2015.

Recommended textbooks

- *Statistical Mechanics* by D.A. McQuarrie, University Science Books, 2000.
- *Computer Simulation of Liquids* by M.P. Allen and D.J. Tildesley, Oxford University Press, 2017.

Prerequisites

Exposure to basic undergraduate thermodynamics, multivariate calculus and elementary probability and statistics. Basic experience with programming (in any language).

Assessment

Your performance will be evaluated through:

- weekly quizzes (25%) that cover required readings,

- 1-2 short programming assignments (25%),
    - These are optional for undergraduate students and can replace the midterm or the final exam.
- a midterm exam* (25%),
    - a different exam will be given to undergraduate and graduate students
- a final exam (25%).
    - a different exam will be given to undergraduate and graduate students

All quizzes and exams are to be worked on independently and show original work. The programming assignments may be worked on in pairs.

***Tentative midterm date: March 10 ***.**

FINAL EXAML: April 25, 3:30pm. CEME-Floor 1-Room 1215.

Course Learning Outcomes

Upon successful completion of this course, students will be able to

- identify and define thermodynamics problems in engineering applications
- apply thermodynamic and statistical thermodynamics principles to gases, solutions, solids and reaction systems
- set up and solve simplified problems using molecular theories relevant to research in modern chemical and biological engineering
- gain an understanding of Monte Carlo simulation techniques
- set up, program, and utilize molecular simulation and visualization tools

Topics to be covered:

- Energy and entropy from the microscopic perspective
    - equilibrium, entropy and probability
    - micrsocopic versus macroscopic perspective
    - Ensemble averages and time average

- Thermodynamic laws and relations
    - fundamental equation
    - first law and reversibility
    - thermodynamic potentials and relations

- Gases, phase equilibrium and condensed phases
    - properties of ideal gases
    - phase equilibrium and ideal solutions and

    - stability
    - non-ideal condensed phases
- Canonical partition functions
    - third law
    - canonical partition function
    - fluctuations
- Classical systems
    - other ensembles
    - chemical equilibrium
- Molecular simulations
    - force fields and intermolecular force
    - statistical averaging
    - visualization

Academic Integrity

The academic enterprise is founded on honesty, civility, and integrity. As members of this enterprise, all students are expected to know, understand, and follow the codes of conduct regarding academic integrity. At the most basic level, this means submitting only original work done by you and acknowledging all sources of information or ideas and attributing them to others as required. This also means you should not cheat, copy, or mislead others about what is your work. Violations of academic integrity (i.e., misconduct) lead to the breakdown of the academic enterprise, and therefore serious consequences arise and harsh sanctions are imposed. For example, incidences of plagiarism or cheating may result in a mark of zero on the assignment or exam and more serious consequences may apply if the matter is referred to the President's Advisory Committee on Student Discipline. Careful records are kept in order to monitor and prevent recurrences. Link to the relevant Calendar section: http://www.calendar.ubc.ca/vancouver/index.cfm?tree=3,286,0,0.

Student Resources

UBC is committed to a community in which every member is respected, included, and celebrated. Taking care of your health and wellbeing is important. UBC Health & Wellness is here to support wellness of mind, body, and spirit, and provides a range of clinical, counselling, and mental health services for students.

The Centre for Accessibility) facilitates educational equity for students with disabilities and chronic medical conditions. If you think you may need academic accommodations to meet the learning outcomes of this course and you have a disability please contact the Centre for Accessibility. If you're not sure that you qualify as having a disability but are concerned, the Centre for Accessibility can help clarify if you are eligible.

Academic Advising empowers students to take ownership of their education at UBC by offering personalized advising services in a supportive environment.

For CHBE-specific issues such as CHBE course registration and planning, you can connect with CHBE Departmental staff (opens in a new window). Drop-in meetings with and advising by CHBE staff is available through Zoom. Staff is available Monday to Friday from 9:00 am to 3:30 pm. You may also email your questions or requests for appointments to undergrad@chbe.ubc.ca. Your email should include your student ID and the specific nature of your enquiry.

For issues beyond CHBE, such as academic concession, late withdrawals, SD exams, and letters of permission/completion, you can reach out to Engineering Academic Services (opens in a new window).

First Nations Longhouse (opens in a new window): The First Nations Longhouse serves as a "home away from home," as well as an academic, social, spiritual, and cultural hub for Indigenous students attending UBC.

Indigenous Liaison for the Faculty of Applied Science (opens in a new window): Catherine McInnis is the designated advisor in Engineering Academic Services for Indigenous students in the Engineering program. faculty member in the position of the Indigenous Liaison for the School of Nursing. You can connect with her through the PD portal or email her directly with three suggested times you are available. Email: catherine.mcinnis@ubc.ca

International Student Advising (opens in a new window) provides advising and resources to assist International students in navigating immigration, health insurance, and settlement matters. Come see an advisor if you have questions about:

UBC's Equity & Inclusion Office provides information about accessible and all-gender washrooms on campus (opens in new window). Information about how to update legal and preferred names (opens in a new window) can be found on the Student Services website. UBC Trans and Non-binary Student Guide (opens in a new window)

Links to an external site. was written in Summer 2020 and describes resources and support on campus for trans and non-binary students.

The Office of the Ombudsperson (opens in a new window) works with all UBC community members to ensure students are treated fairly and can learn, work, and live in a fair, equitable and respectful environment. If you have concerns about relevant UBC policies and/or processes, an Ombuds Officer can identify and explain policies and guide you in exploring options for directly and effectively dealing with your concerns.

The Sexual Assault Support Center (SASC) (opens in a new window)

Links to an external site. is committed to the education, support, and empowerment of people of all genders who are survivors of sexualized violence, as well as their friends and family.