



## CHM 1480: STATISTICAL MECHANICS

### Winter 2024 Course Syllabus

#### I TEACHING TEAM

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##### INSTRUCTOR

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Office: LM420D

Student hours: Tue. 1:30-2:30 pm in LM 420D

##### MARKER

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#### II COURSE OVERVIEW

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##### COURSE DESCRIPTION:

Equilibrium statistical mechanics with applications to molecular dynamics; an introduction to nonequilibrium statistical mechanics

##### STUDENT LEARNING OUTCOMES:

Knowledge of the foundations of statistical mechanics and its application to gas phase and liquid phase; familiarity with computer molecular dynamics simulations; understanding the integration of statistical mechanics with classical thermodynamics and quantum mechanics; communication of scientific ideas and results; basic scientific programming.

##### PREREQUISITE COURSE(S):

Check Chemistry/A&S information

##### READINGS:

**Suggested textbook:** Tuckerman, Statistical Mechanics: Theory and Molecular Simulation, Oxford

### III COURSE ORGANIZATION

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#### COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

Dates (rough)	UNIT/WEEK	TOPICS
Jan 11-18	1-2	Introduction: classical mechanics; relation between statistical mechanics and thermodynamics; microscopic versus macroscopic quantities; average values in statistical mechanics
Jan 25-Feb 8	3-5	Ensemble theory: time averages versus ensemble averages; microcanonical, canonical and grand canonical ensembles; fluctuations in different ensembles The Ising model
Feb 15	6	Applications to liquids and condensed phases: discussion of reduced distribution functions; radial distribution function; potential of mean force
Feb 22	7	Grand canonical ensemble and Monte Carlo
March 7	8	Quantum ensembles: Quantum ideal gases, Fermi-Dirac and Bose-Einstein statistics
March 14-21	9-10	Nonequilibrium statistical mechanics: Brownian motion theory; Langevin and Fokker-Planck equations; correlation function expressions for transport properties; linear response theory.
March 28	11	Master equations + students' presentations
April 04	12	Students' presentations

### IV EVALUATION/GRADING SCHEME

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**5 HW sets** = 70%

Penalty: 2 points per day are taken for late submission. Please contact me ahead of time if you require accommodations.

**10 mins. class presentation** = 10%

**Exam** = 20%

- Submit on Quercus
- Assignments will require you to perform simple simulations (recommended with MATLAB or Python).
- UofT students can use Matlab Online or download and install MATLAB to their personally-owned machines free of charge. You do not need to install Matlab—Matlab Online is perfectly suitable.

- This is a cross-listed course (CHM427/CHM1480). HW sets and the final exam for *graduate students* will require stronger math and coding technical skills than those for undergraduate students.

#### ASSESSMENT DATES & MARK BREAKDOWN:

Assignment	From	Due date	Weight/100
Set 1	Jan 11	Jan 25	15
Set 2	Jan 25	Feb 08	15
Set 3	Feb 08	Feb 29	15
Set 4	Feb 29	March 21	15
Set 5	March 21	April 4	10
Class presentation	March 31 April 04		10
Exam		Exam period	20

These are **tentative** dates, to be modified according to teaching pace. Please follow announcements in class and on the portal.

**IMPORTANT:** if an unexpected technical issue occurs with a university system (e.g., Quercus services, network outage) that affects availability or functionality, it may be necessary to revise the timing or weighting of the two quizzes.

## V COURSE POLICIES

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- Each member of this course is expected to maintain a
  - professional and respectful attitude during all course activities, including classes, laboratories, tutorials, and online activity.
  - personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met.
  - collection of notes recorded independently based on concepts covered in course activities (students registered with Accessibility Services requiring a class note-taker will have access to this accommodation)
  - familiarity with the university policy on Academic Integrity (overleaf)
- The University of Toronto is committed to equity, human rights, and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. As a Course Instructor, I will neither condone nor tolerate behaviour that undermines the dignity or self-esteem of any

individual in this course and wish to be alerted to any attempt to create an intimidating or hostile environment. It is our collective responsibility to create a space that is inclusive and welcomes discussion. Discrimination, harassment and hate speech will not be tolerated. If you have any questions, comments, or concerns, we encourage you to reach out to the staff in our Equity Offices.

- Process for signaling course absences and requesting make-up tests or other missed pieces of work.

If you are absent from your studies due to illness or other reasons and unable to complete course work (e.g., a term test or an assignment) then a piece of written documentation is required. The following four items are the recognized forms of documentation:

1. Absence Declaration via ACORN (please note the circumstances under which an absence declaration can and cannot be submitted)
2. U of T Verification of Illness or Injury Form
3. College Registrar's letter
4. Letter of Academic Accommodation from Accessibility Services

Students who complete the ACORN Absence Declaration form must additionally contact me to discuss their situation within five business days of the missed piece of work. This is essential action for any consideration to be granted.

For extended absences and for absences due to non-medical reasons, make sure to contact your College Registrar's Office. They can help you decide between a request for an extension or other types of academic consideration.

If you suspect or know that you have a disability that is affecting your studies, learn about the services and supports available through Accessibility Services. A disability can be physical disability, sensory disability, a learning disability, mental health disorder or a short-term disability like an injury. If you are not sure whether you have a disability, you can confidentially contact Accessibility Services with your questions.

- **Information regarding used of artificial intelligence tools:**
- The use of generative artificial intelligence tools and apps is strictly prohibited in all course assignments unless explicitly stated otherwise by the instructor in this course. This includes ChatGPT and other AI writing and coding assistants. Use of generative AI in this course may be considered use of an unauthorized aid, which is a form of cheating.
- **Communication with instructor:** I will respond to email within 24 hrs. on weekdays.
- **Privacy language and appropriate use of course materials:** See the syllabus "Copyright" section.

- **Policy for reweighting due to missed pieces of academic work:** For students missing one piece for a valid reason, the missed weight will be divided between other HW assignments and the Exam. For students missing two or more pieces for valid reasons, the mark for the missing pieces will be replaced by a two-hour assessment to be written in-person.

## VI TECHNOLOGY REQUIREMENTS

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- This course requires the use of computers, and technical issues are possible. When working on a piece of academic work, students are responsible for scheduling enough time to allow for reasonable delays due to technical difficulties to be overcome, so such issues will not be acceptable grounds for deadline extension. Particularly, maintaining an up-to-date independent backup copy of your work is strongly recommended to guard against hard-drive failures, corrupted files, lost computers, etc.

## VII INSTITUTIONAL POLICIES & SUPPORT

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### ACADEMIC INTEGRITY

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University of Toronto's Code of Behaviour on Academic Matters ([governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019](http://governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019)) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In assignments:

1. Using someone else's ideas or words without appropriate acknowledgement.
2. Submitting your own work in more than one course without the permission of the instructor.
3. Making up sources or facts.
4. Obtaining or providing unauthorized assistance on any report. **Please note that the use of websites (such as Chegg.com or the course discussion board) to post laboratory report material/questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student**

## **Academic Integrity office.**

On quizzes and term tests:

1. Using or possessing unauthorized aids. **Please note that the use of websites (such as Chegg.com or the course discussion board) to post quiz/term test questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.**
2. Looking at someone else's answers or collaborating/discussing answers during a quiz or term test.
3. Misrepresenting your identity.

In general academic work:

1. Falsifying institutional documents or grades.
2. Falsifying or altering any documentation required by the University.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see [www.academicintegrity.utoronto.ca/](http://www.academicintegrity.utoronto.ca/)).

## **COPYRIGHT**

If a student wishes to copy or reproduce class presentations, course notes or other similar materials provided by instructors, he or she must obtain the instructor's written consent beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited.

## **ACCESSIBILITY**

Students with diverse learning styles and needs are extremely welcome in this course. The University of Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact [Accessibility Services](#) as soon as possible.

## **NEEDS**

## **ACCOMMODATIONS FOR RELIGIOUS OBSERVANCES**

Following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of an assignment, tutorial, class or laboratory session. Students must inform the instructor **before** the session/assignment date to arrange accommodations.

## **ADDITIONAL SERVICES & SUPPORT**

The following are some important links to help you with academic and/or technical service and support:

- General student services and resources at [Student Life](#)

- Full library service through [University of Toronto Libraries](#)
- Resources on conducting online research through [University Libraries Research](#)
- Resources on academic support from the [Academic Success Centre](#)
- Learner support at the [Writing Centre](#)
- Information for [Quercus Support](#)

### **ACKNOWLEDGEMENT OF TRADITIONAL LANDS**

We wish to acknowledge this land on which the University of Toronto operates. For thousands of years, it has been the traditional land of the Huron-Wendat, the Seneca and, most recently, the Mississaugas of the Credit River. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and we are grateful to have the opportunity to work on this land.