



Chemistry
UNIVERSITY OF TORONTO

CHM 427: STATISTICAL MECHANICS

2023 Course Syllabus

I TEACHING TEAM



INSTRUCTOR

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MARKER

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II COURSE OVERVIEW

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.

III COURSE ORGANIZATION

Class: Thur. 4-6 pm LM123

Student Office hours:

- Tue 4-4:30pm in LM 420D
- Tue 4:30-5pm over zoom (see Quercus for meeting ID)
- Contact me by email to set a different time

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

Email: Please communicate with me using UofT emails; please write CHM427/1480 in the subject line

COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

Dates (rough)	UNIT/WEEK	TOPICS
Jan 1-15	1-2	Introduction: classical mechanics; relation between statistical mechanics and thermodynamics; microscopic versus macroscopic quantities; average values in statistical mechanics
Jan 15-Feb 10	3-5	Ensemble theory: time averages versus ensemble averages; microcanonical, canonical and grand canonical ensembles; fluctuations in different ensembles
Feb 10-28	6-7	Applications to liquids and condensed phases: discussion of reduced distribution functions; radial distribution function; potential of mean force
March 1-15	8-9	Quantum ensembles: Quantum ideal gases, Fermi-Dirac and Bose-Einstein statistics
March 15-31	10-11	Nonequilibrium statistical mechanics: Brownian motion theory; Langevin and Fokker-Planck equations; correlation function expressions for transport properties; linear response theory.
	1-12	Nonequilibrium statistical mechanics: Brownian motion theory; Langevin and Fokker-Planck equations; correlation function expressions for transport properties; linear response theory.

IV EVALUATION/GRADING SCHEME

5 HW sets = 75% (penalty: 2 points/15 per day are taken for late submission.
Please contact me ahead of time if you require accommodations)

10 mins. class presentation = 10%

Take-home test = 15%

- Submit on Quercus
- Assignments will require you to perform simple simulations (recommended with MATLAB or Python). Assistance-guidance with basic Matlab will be provided.
- 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.

ASSESSMENT DATES & MARK BREAKDOWN:

Assignment	From	Due date	Weight/100
Set 1	Jan 12	Jan 26	15
Set 2	Jan 26	Feb 09	15
Set 3	Feb 09	March 02	15
Set 4	March 02	March 16	15
Set 5	March 16	April 0	15
Class presentation	March 31	TBD	10
Take home test	Last week of semester or	Exam period	15

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

We will not have a class on April 06. Suggested makeup days are March 31, April 3,4, or 10.

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 assignments.

V COURSE POLICIES

- Each member of this course is expected to maintain a:
 - (i) professional and respectful attitude during all course activities, including classes, laboratories, tutorials and online activity.
 - (ii) personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met.
 - (iv) familiarity with the university policy on Academic Integrity
- 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.
- Communication with instructor: I will respond to email within 24 hrs. on weekdays.
- Policy for late assignment submissions: penalty of 2 points/15 per day are taken for late submission. Contact me in advance for accommodations.
- Submission methods (use Quercus/papers).

VI TECHNOLOGY REQUIREMENTS

- 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

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) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In home 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 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/).

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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 NEEDS

Students with diverse learning styles and needs are 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.

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](#)

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.