Chemistry
UNIVERSITY OF TORONTO

CHM 328H: Modern Physical Chemistry

Course Syllabus: Winter 2023

I TEACHING TEAM

INSTRUCTOR
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Student hours: at office after class [4-5 pm Tue & Thu]

Prof. von Lilienfeld is the inaugural Clark Chair in Advanced materials at University of Toronto and at the Vector Institute. He is also a Canada CIFAR AI Chair at the Vector Institute. Previously he has held professorships at various European universities (Physics, University of Vienna (2020-2022); Physical Chemistry, University of Basel (2013-2020); Computational Chemistry, University of Brussels (2016)). Over the years he has been teaching undergraduate courses on `Introduction to physical chemistry', `Physical chemistry IV: Electronic structure', `Physical Chemistry I: Thermodynamics', `Quantum chemistry: Density Functional Theory', and `Theoretical Physics I: Classical Mechanics'. Research in his lab deals with first principles based studies of chemical compound space using quantum mechanics, statistical mechanics, and machine learning. Recordings of some of his research presentations and teaching playlists can be found at his youtube channel Prof von Lilienfeld - YouTube. Personal postings (mostly related to academic research and teaching activities) can be found at Anatole von Lilienfeld (@ProfvLilienfeld) / Twitter

TEACHING ASSISTANT
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Office: Myhal, room 715
Student hours: after tutorial [2-3 pm Wed]

II COURSE OVERVIEW

COURSE DESCRIPTION:
In CHM328 macroscopic phenomena are described from a microscopic point of view and to build a bridge between the quantum mechanics of atoms and molecules studied in CHM223 and CHM326 and the thermodynamic treatment of macroscopic systems studied in CHM222 and CHM151/CHM135.
CHM328 provides an introduction to statistical thermodynamics which is a branch of physical chemistry that uses statistical methods to explain the macroscopic behavior of chemical systems based on microscopic arguments. By bridging the gap

between the microscopic and macroscopic views of matter, statistical thermodynamics describes how the behavior of individual particles at the microscopic level can be related to the macroscopic properties of a system, such as its temperature, pressure, and volume. This understanding is crucial for understanding, predicting and controlling the behavior of materials in a wide range of applications, including engineering, materials science, biology, and chemistry.

STUDENT LEARNING OUTCOMES:
By the end of this course, students will be able to:

- Understand the fundamentals of statistical thermodynamics
- Discuss the role of the partition function
- Explain and describe how to predict macroscopic properties
- Communicate ideas from statistical thermodynamics
- Perform derivations and calculations related to important properties

PREREQUISITE COURSE(S):
This course assumes you have a basic understanding of elementary physics and physical chemistry. The language used is mathematical and involves multivariable calculus. A modest level of mathematical sophistication is required for the success in the course. The pre-requisites for the course are: CHM222 and CHM223.

READINGS:
Recommended: Physical Chemistry by Ira N. Levine

III COURSE ORGANIZATION

This course is organized in content by week. In addition to the lectures and recommended reading, for each week, there will be problem sets (some marked) for discussion in tutorials. Students are expected to attend all classes, work through problem sets, and to attend tutorials.

COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

DATES	UNIT/WEEK	TOPICS
Jan 09	1	Introduction
Jan 16	2	Partition function & canonical ensemble
Jan 23	3	Calculating state functions
Jan 30	4	Translatory, spin, and rotational DOFs
Feb 06	5	Vibrational and electronic DOFs
Feb 13	6	Recap
Feb 20		
Feb 27	7	Equilibrium constants
Mar 06	8	Transition state theory
Mar 13	9	Classical statistical thermodynamics
Mar 20	10	Density operator
Mar 27	11	Solids
Apr 03	12	Recap

TUTORIAL OBJECTIVES:
During the tutorials the TA will discuss how to solve the problem sets (marked and unmarked). Problem sets will be provided in person after each Thursday lecture. The problem sets serve as proxies to term test and final examination. Consequently, active participation and continued attendance of all course participants is strongly recommended.

IV EVALUATION/GRADING SCHEME

OVERVIEW:
Marked Problem sets (x5): 20%
Summaries: 10%
Questions: 10%
Term test: 10 or 20%
Final examination (in-person): 50 or 40%

ASSESSMENT DATES & MARK BREAKDOWN:
1. Five problem sets (each 4%): To be submitted via Quercus **before** the tutorial begins.

2. Summaries (10%*): Briefly summarize materials taught in the preceding lecture.

3. Questions (10%*): Answer questions regarding preceding lecture's materials.

4. Term Test (10 or 20% whatever is higher in combination with final examination grade**, Tuesday 7th February): 50 minutes, to be written during regularly scheduled class time.

5. Final examination (50 or 40%, whatever is higher in combination with term test grade**, 2 hours, date to be announced but during final examination period April 11 - 28)

Students who are absent from class for any reason (e.g., COVID-19 illness, other illness or injury, family situation) and who require consideration for missed academic work should report their absence through the online absence declaration. The declaration is available on ACORN under the "Profile and Settings" menu. A student who misses any form of evaluation must additionally contact both, instructor and tutor, via email with a screenshot of their ACORN absence declaration WITHIN ONE WEEK to discuss their situation. This is a requirement to receive consideration for the missed evaluation

*At the beginning of each lecture, one or two students will be selected at random and asked to provide a brief summary of the preceding lecture. Thereafter, and during the course, the instructor will ask questions to other students selected at random. Resulting grades will be communicated after class to the corresponding students by email. The grades will be assigned according to the following rubric:

1. Understanding:

- Inadequate: Lacks basic understanding of the material and cannot apply it to physical chemistry examples.
- Marginal: Demonstrates basic understanding of the material, but has difficulty exemplifying it for examples in physical chemistry.
- Adequate: Demonstrates good understanding of the material, but could improve the discussion of physical chemistry implications.
- Good: Demonstrates deep understanding of the material, including its relevance to physical chemistry.
- Excellent: Demonstrates thorough and nuanced understanding of the material, including its application to physical chemistry and broader implications.

2. Engagement:

- Inadequate: Does not participate in discussions or engage with classmates.
- Marginal: Contributes minimally to discussions and could benefit from more engagement.
- Adequate: Participates meaningfully in discussions, but could be more actively engaged with classmates.
- Good: Actively engages with classmates, asking and answering questions and contributing to discussions with substantial content.
- Excellent: Not only actively engages with classmates, but also initiates and leads discussions, assistant towards the emergence of a collaborative and engaging learning environment.

3. Time Management:

- Inadequate: Goes significantly over allotted time and disrupts flow of content.
- Marginal: Goes over allotted time, but does not significantly disrupt the course.
- Adequate: Stays within allotted time, but could improve time management skills.
- Good: Stays within allotted time and effectively manages presentation.
- Excellent: Stays within allotted time and delivers a well-organized and coherent presentation.

For students missing the summary and/or questions, the corresponding grade will be interpolated as the weighted average of marked problem sets, term test, and final examination.

**For students missing the term test, the weight of the test will be added to the final examination.

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 marked problem sets.

V COURSE POLICIES

- Students are strongly encouraged to take notes using pen and paper. The use of any mobile devices such as laptops, tablets, calculators, or cell-phones is strictly prohibited during class.
- 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.

(iii) 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)

(iv) 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. The Course Instructor 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: Preferably during class or office-hours. If in person communication is impossible for whatever reason one can send an email. The email will be answered within 48 hrs. on weekdays. The subject line must begin with ''CHM328:" …
- Privacy language and appropriate use of course materials: For additional information, see the syllabus "Copyright" section.
- Policy for late submissions: Solutions to marked problem sets that are handed in too late (i.e. after the corresponding tutorial explaining the solutions started) will be graded as a fail.
- Problem sets should be handed over to the tutor at the beginning of the tutorial, or by following information provided during the lecture or the tutorials .
- Legitimate requests for re-grading of course work should be addressed to the instructor. Course absences or failure to submit solutions to marked problems (only for valid reasons) must also be communicated to the tutor as soon as possible.

VI TECHNOLOGY REQUIREMENTS

- Students are strongly encouraged to make use of computers and literature when working on problem sets and when revisiting their notes taken. Consequently, 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.
- Specific guidance from the U of T Vice-Provost, Students regarding student technology requirements is available here: https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/
- Advice for students more broadly regarding online learning is available here: https://onlinelearning.utoronto.ca/getting-ready-for-online/

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:

On term tests:

1. Using or possessing unauthorized aids. **Please note that the use of websites (such as Chegg.com) to post 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 and copying someone else's answers or collaborating/discussing answers during a 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/).

COPYRIGHT

This course, including your participation, might be recorded on video and might be made available to students in the course for viewing remotely. Course videos and materials belong to your instructor, the University, and/or other source depending on the specific facts of each situation, and are protected by copyright. In this course, you are permitted to download session videos and materials for your own academic use, but you should not copy, share, or use them for any other purpose without the explicit permission of the instructor. For questions about recording and use of videos in which you appear please contact your instructor.

The unauthorised use of any form of device to audiotape, photograph, video-record or otherwise reproduce lectures, course notes or teaching materials provided by instructors is covered by the Canadian Copyright Act and is prohibited. Students must obtain prior written consent to such recording. In the case of private use by students with disabilities, the instructor's consent must not be unreasonably withheld.

Students may not create audio or video recordings of classes with the exception of those students requiring accommodation for a disability, who should speak to the instructor prior to beginning to record lectures. Students creating unauthorized audio recording of lectures violate an instructor's intellectual property rights and the Canadian Copyright Act. Students violating this agreement will be subject to disciplinary actions under the Code of Student Conduct.

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
- 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.