CHM427 and Graduate Course CHM1480: Statistical Mechanics

Contact info
Course coordinator and Instructor (weeks 1-4): Prof. Dvira Segal
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Course Instructor (weeks 5-12): Dr. Chong Sun, chong.sun@utoronto.ca

Please use UofT emails; **please write CHM427/CHM1480 in the subject line**

Classes: Thur. 4-6 pm LM123
Office Hours Segal: Tue. 4-5 pm - or email me to set an alternative time.
Chong Sun: Mon. 2-3 pm.
Zoom link will be provided on Quercus.

Prerequisite: CHM326H1, CHM328H1

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

Marking Scheme
5 HW sets = 75% (penalty: 2 points/16 **per day** are taken for late submission)
10 mins. class presentation = 10%
Take-home test= 15%.

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

Assignments	From	Due date	weight/100
set 1	Jan 13	Jan 27	15
set 2	Jan 27	Feb 10	15
set 3	Feb 10	March 03	15
set 4	March 03	March 17	15
set 5	March 17	April 07	15
class presentation (last class)	March 31	April 07	10
Take home test	Last week of semester or	exam period	15

Sets will offer some flexibility in selecting problems to solve.
These are tentative dates, to be modified according to teaching pace. Please follow announcements in class and on the portal.

Academic Integrity
Please click, read and act with honesty: Academic Integrity at U of T and Code of behaviour of academic matters

Offences include (but are not limited to): Using ideas of another person without acknowledgement; Submitting your work in more than one course without the approval of the instructor; Obtaining or providing unauthorized assistance on any assignment. Misconduct will be reported to the Associate Chair, Undergraduate/Graduate Studies

Copyright
Link to copyright-considerations at UofT
Lectures will be recorded on video and will be shared on Quercus with students in the course.

Course videos and materials belong to your instructor, the University, and/or other sources depending on the specific facts of each situation and are protected by copyright. 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.

Suggested textbook
Tuckerman, Statistical Mechanics: Theory and Molecular Simulation, Oxford
Class notes will be provided. No need to purchase the book
Syllabus

The course will cover basic aspects of equilibrium and nonequilibrium statistical mechanics.

1. Introduction: classical mechanics; relation between statistical mechanics and thermodynamics; microscopic versus macroscopic quantities; average values in statistical mechanics (week 1-2)

2. Ensemble theory: time averages versus ensemble averages; microcanonical, canonical and grand canonical ensembles; fluctuations in different ensembles (week 3-5)

3. Applications to liquids and condensed phases: discussion of reduced distribution functions; radial distribution function; potential of mean force (week 6-7)

4. Quantum ensembles: Quantum ideal gases, Fermi-Dirac and Bose-Einstein statistics (week 8-9)

5. Nonequilibrium statistical mechanics: Brownian motion theory; Langevin and Fokker-Planck equations; correlation function expressions for transport properties; linear response theory. (week 10-11)

6. Numerical simulations: Molecular dynamics in various ensembles; Nose Hoover thermostat; Langevin thermostat; Monte Carlo (embedded)

Announcements
Home assignments, solutions, and other important announcements will be posted on the CHM427-CHM1480 website on Quercus. It is your responsibility to regularly check postings on Quercus.