**CHM1480: Statistical Mechanics**

**Contact info**
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Please use UofT emails; **please write CHM1480 in the subject line**

**Classes:** Thur. 4-6 pm LM123
**Office Hours:** Tue. 4-5 pm - or email me to set an alternative time.
LM420D or on Zoom (link will be provided on Quercus).

**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/15 **per day** are taken for late submission. Please contact me ahead of time if you require accomodations)
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-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**. MATLAB (You do not need to install Matlab— Matlab Online is perfectly suitable)

| Assignments | From | Due date | weight/100 |
|---|---|---|---|
| set 1 | Jan 12 | Jan 26 | 15 |
| set 2 | Jan 26 | Feb 9 | 15 |
| set 3 | Feb 9 | March 02 | 15 |
| set 4 | March 02 | March 16 | 15 |
| set 5 | March 16 | April 06 | 15 |
| class presentation (last 2 classes) | March 31 | TBD | 10 |
| Take home test (2 hours) | 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.

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

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

of academic matters

Offenses 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

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

**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 Quercus. It is your responsibility to regularly check postings on Quercus.