# CHEM 630P (CHEM 498P): Statistical Mechanics
# Syllabus for Summer 2009 Term

## GENERAL INFORMATION

Statistical Mechanics is the formal study of how the macroscopic properties of a complex system emerge from the microscopic properties of their molecular constituents. In recent years, with the availability of ever more powerful computers, the field has expanded into many new areas of application—from material science to biochemistry—and is quickly becoming one of the most important conceptual tools for establishing a connection between macroscopic observations and the underlying physicochemical processes. This 3-credit course is intended to provide the student with an understanding of the principles and techniques of modern statistical mechanics and with the practical skills to implement them.

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## COURSE OUTLINE

The following topics will be covered: FUNDAMENTALS: Probability theory, Classical mechanics, Review of thermodynamics, Equilibrium ensembles and fluctuations; IDEAL SYSTEMS: Classical and quantum ideal gases, [Mixtures of ideal gases]; REAL SYSTEMS: Distribution functions, [Integral equation theories], Molecular dynamics; PHASE TRANSITIONS: Mean field theory, [Renormalization group theory], Monte Carlo methods; NONEQUILIBRIUM STATISTICAL MECHANICS: Langevin equation, [Fokker-Plank equation], Linear response theory.

## EVALUATION

The final grade for the course is composed as follows: **50% for the mini-project and 50% for the final comprehensive exam**. The mini-project will be evaluated on two oral presentations and a written report. The oral presentations will be evaluated by both the students and the instructor (half of the grade will come from the instructor evaluation, and half from the students evaluations).

## MINI-PROJECT

The mini-project will consist of the following:
- an oral presentation of the theoretical background for the project (in a lecture/journal club format);
- the implementation of a computer program to generate the results;
- a written report explaining the theory and its computer implementation, presenting the results, and discussing their significance and validity;
- an oral presentation of the results (in a talk format).

The topics will be assigned to the students no later than Friday, May 15. The first oral presentations will be on May 27 and 28, and the second presentations will be on June 16. A detailed outline of the report should be submitted electronically **no later than Friday, May 29**. The final report itself should be submitted both electronically and as a hard copy **no later than Friday, June 12**.

**FINAL COMPREHENSIVE EXAM**

The final comprehensive exam will be a closed-book, written exam based on two or three scientific articles given to the students about one week prior to the examination. The students will be expected to fully understand the content of these articles (the phenomena studied, the results presented, and the theories and methods used) and be able to provide a critical evaluation of them.

**PLAGIARISM AND OTHER FORMS OF ACADEMIC DISHONESTY**

The academic code of conduct can be found in the Graduate Calendar, at *http://graduatestudies.concordia.ca/formsandpublications/graduatecalendar/current/PartVII/a-academicintegrity.pdf*. Any form of unauthorized collaboration, cheating, copying or plagiarism found in this course will be reported and the appropriate sanctions applied. Ignorance of these regulations is no excuse and will not result in a reduced sanction in any case where academic misconduct is observed. Students can find more resources on academic integrity at *http://provost.concordia.ca/academicintegrity/*.

**CALENDAR**

(Please note that this calendar may change as the term proceeds.)

| **Date** | | **Topics** |
|---|---|---|
| May 6 | Lecture | Fundamentals: Probability theory |
| May 7 | Lecture | Fundamentals: Classical mechanics, Review of thermodynamics |
| May 12 | Lecture | Fundamentals: Equilibrium ensembles and fluctuations |
| May 14 | Lecture | Fundamentals: Equilibrium ensembles and fluctuations (contd.) |
| May 19 | Lecture | Ideal systems: Classical and quantum ideal gases |
| May 20 | Lecture | Real systems: Distribution functions |
| May 26 | Lecture | Real systems: Molecular dynamics |
| **May 27** | **Presentations** | **First oral presentations** |
| **May 28** | **Presentations** | **First oral presentations (contd.)** |
| **May 29** | **–** | **Due date for the detailed outline (PDF)** |
| June 4 | Lecture | Phase transitions: Mean field theory |
| June 9 | Lecture | Phase transitions: Monte Carlo methods |
| June 11 | Lecture | Nonequilibrium: Langevin equation, Linear response theory |
| **June 12** | **–** | **Due date for the written report (PDF + hard copy)** |
| **June 16** | **Presentations** | **Second oral presentations** |
| **TBA** | | **Final comprehensive exam** |