Statistical Mechanics
CHEM/ENCH 412

Instructor: Natalie Cann

Contact Information:

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Office Hours:

Wednesday 10:30-12:00
If you cannot drop by at this time, please send an Email to set an alternate date/time to meet.

Lectures:

Lecture times: Monday 10:30-11:30
Wednesday 9:30-10:30
Friday 8:30-9:30
Lecture location: Jeffery 110

onQ site

The site includes the assignments, your marks, the formula and data sheets for the midterm and exam, and other information.

Intended Student Learning Outcomes

At the end of CHEM 412, students will be able to…

- Evaluate bulk properties based on knowledge of the partition function.
- Discuss trends in properties (equilibrium constants, heat capacities, etc) based on knowledge of partition functions.
- Interconnect previous knowledge in quantum mechanics, thermodynamics, and spectroscopy using statistical mechanics principles.
- Apply statistical mechanical principles to a selection of topics in physical chemistry.
- Explain the statistical mechanical underpinnings of modern simulations.

Course Outline

A. Fundamentals

Chapter 1:

- General philosophy of statistical mechanics (going from knowledge of individual molecules to Avogadro's number of molecules)
- General concepts: ensembles, mechanical and non-mechanical properties
- Probabilities

Chapter 2:

- Boltzmann statistics
- Fermi-Dirac statistics (for fermions)
- Bose-Einstein statistics (for bosons)

B. Applications

Chapter 3:	Crystals; the Einstein model and the Debye model
Chapter 4:	Gases; electronic, nuclear, rotation, vibration, translation, and quantum effects.
Chapter 5:	Equilibrium and kinetics, including isotopic exchange and gas phase reactions.
Chapter 6:	Interfaces; the tight-attachment model, the mobile-attachment model, and the in-between situation.
Chapter 7:	Quantum statistics; low temperatures, electrons in metals, the classical limit, and molecular simulations.

Textbooks/Readings

- Statistical Mechanics by McQuarrie.
- An Intro to Statistical Thermodynamics by Hill.

Neither text is *required* for the course. Copies of both texts are available in the library. Also, I have several copies of the McQuarrie text available to borrow. If you would like to purchase a text, I suggest the Hill book.

Marking Scheme

4 assignments:	4 x 5%	20%	Due: Feb 2, Feb 16, March 16, March 30.
1 midterm:	1 x 30%	30%	March 2nd.
1 final exam:	1 x 50%	50%	TBD

Grading Method

All components of this course will receive numerical percentage marks. The final grade you receive for the course will be derived by converting your numerical course average to a letter grade according to Queen's Official Grade Conversion Scale:

Queen's Official Grade Conversion Scale

Grade	Numerical Course Average (Range)
A+	90-100
A	85-89
A-	80-84
B+	77-79
B	73-76
B-	70-72
C+	67-69
C	63-66
C-	60-62
D+	57-59
D	53-56
D-	50-52
F	49 and below

Calculator Policy

As noted in Academic Regulation 9.2, Calculators acceptable for use during quizzes, tests and examinations are intended to support the basic calculating functions required by most Arts and Science courses. For this purpose, the use of the Casio 991 series calculator is permitted and is the only approved calculator for Arts and Science

students. This calculator sells for around $25 at the Queen's Campus Bookstore, Staples and other popular suppliers of school and office supplies.

Academic Integrity

Academic Integrity is constituted by the six core fundamental values of honesty, trust, fairness, Respect, responsibility and courage (see www.academicintegrity.org). These values are central to the building, nurturing and sustaining of an academic community in which all members of the community will thrive. Adherence to the values expressed through academic integrity forms a foundation for the "freedom of inquiry and exchange of ideas" essential to the intellectual life of the University (see the Senate Report on Principles and Priorities http://www.queensu.ca/secretariat/policies/senate/report-principles-and-priorities).

Students are responsible for familiarizing themselves with the regulations concerning academic integrity and for ensuring that their assignments conform to the principles of academic integrity. Information on academic integrity is available in the Arts and Science Calendar (see Academic Regulation 1 http://www.queensu.ca/artsci/academic-calendars/regulations/academicregulations/regulation-1), on the Arts and Science website (see http://www.queensu.ca/artsci/academics/undergraduate/academic-integrity), and from the instructor of this course. Departures from academic integrity include plagiarism, use of unauthorized materials, facilitation, forgery and falsification, and are antithetical to the development of an academic community at Queen's. Given the seriousness of these matters, actions which contravene the regulation on academic integrity carry sanctions that can range from a warning or the loss of grades on an assignment to the failure of a course to a requirement to withdraw from the university.

Turnitin Statement

Queen's University has partnered with the third-party application Turnitin to help maintain our standards of excellence in academic integrity. Turnitin is a suite of tools that provide instructors with information about the authenticity of submitted work and facilitates the process of grading. Submitted files are compared against an extensive database of content, and Turnitin produces a similarity report and a similarity score for each assignment. A similarity score is the percentage of a document that is similar to content held within the database. Turnitin does not determine if an instance of plagiarism has occurred. Instead, it gives instructors the information they need to determine the authenticity of work as a part of a larger process.

Copyright of Course Materials

All materials associated with this course are copyrighted. This includes in-class handouts, Emailed information, and all documents and information provided on the course Moodle site. These course materials are for the sole use of students registered in the course. These materials shall not be distributed or disseminated to anyone other than students registered in this course. Failure to abide by these conditions is a breach of copyright, and may also constitute a breach of academic integrity under the University Senate's Academic Integrity policy statement.

Accessibility Statement

Queen's is committed to an inclusive campus community with accessible goods, services, and facilities that respect the dignity and independence of persons with disabilities. Course materials are available in an accessible format or with appropriate communication supports upon request.

Please contact Meredith Richards in the Department of Chemistry in one of the following ways:

Email: ugadm@chem.queensu.ca
Phone: 613-533-6000 extension 75518
In person: Chernoff 200

Accommodations Statement

Queen's University is committed to achieving full accessibility for persons with disabilities. Part of this commitment includes arranging academic accommodations for students with disabilities to ensure they have an equitable opportunity to participate in all of their academic activities. If you are a student with a disability and think you may need accommodations, you are strongly encouraged to contact Student Wellness Services (SWS) and register as early as possible. For more information, including important deadlines, please visit the Student Wellness website at: http://www.queensu.ca/studentwellness/accessibility-services/

Academic Considerations for Students in Extenuating Circumstances

The Senate Policy on Academic Consideration for Students in Extenuating Circumstances (http://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslcwww/files/files/policies/ExtenuatinCircumstancesPolicyFinal.pdf) was approved in April, 2017. Queen's University is committed to providing academic consideration to students experiencing extenuating circumstances that are beyond their control and which have a direct and substantial impact on their ability to meet essential academic requirements. The Faculty of Arts and Science is developing a protocol to provide a consistent and equitable approach in dealing with requests for academic consideration for students facing extenuating circumstances, which will be posted on the Faculty of Arts and Science website in Fall, 2017.

Location and Timing of Final Examinations

As noted in Academic Regulation 8.2.1, "the final examination in any class offered in a term or session (including Summer Term) must be written on the campus on which it was taken, at the end of the appropriate term or session at the time scheduled by the Examinations Office." The exam period is listed in the key dates prior to the start of the academic year in the Faculty of Arts and Science Academic Calendar and on the Office of the University Registrar's webpage. A detailed exam schedule for the Fall Term is posted before the Thanksgiving holiday; for the Winter Term it is posted the Friday before Reading Week, and for the Summer Term the window of dates is noted on the Arts and Science Online syllabus prior to the start of the course. Students should delay finalizing any travel plans until after the examination schedule has been posted. Exams will not be moved or deferred to accommodate employment, travel /holiday plans or flight reservations.