Welcome to CHEM 4444B!

Instructor  Dr. Styliani Constas, Room 071-Chemistry Building, ext. 86338

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Lecture times  Monday, Wednesday, Friday 9:30-10:30 am in ChB 115.

Office hours  Monday 4:00 pm -5:00 pm, Wendsday 4:00 pm-5:00 pm or by appointment

Course website  http://owl.uwo.ca/portal

Notice from the Registrar  Unless you have either the prerequisites for this course or written special permission from your Dean to enroll in it, you will be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites, which are Chemistry 3374A/B or the former Chemistry CHEM 3384F/G.

Course Learning Outcomes

Breadth and Depth of Knowledge:  Be able to describe the fundamental scientific principles of the physical chemistry using the laws that govern the motions of molecules and apply these principles in assignments, discussions on/off line.

Knowledge of Methods:  Obtain problem-solving skills in physical chemistry by assignments, on/off-line discussions and lecture materials.

Application of Knowledge:  Be able to apply the knowledge in order to predict and rationalize the physical and chemical properties of systems.

Communication:  Be able to prepare logical and concise written reports via training in quizzes and assignments.

Awareness of Knowledge Limits:  Recognize assumptions and limitations in the scientific models and their possible impact on the results by training on case studies, lectures, assignments.
Autonomy and Professional Capacity: (1) Be able to work productively and collaboratively as a team member. (2) Evaluate the potential impact chemistry may have in society, health and environment.

Course Textbook  Lecture Notes

Helpful books that are close to the material of the course are any of the following:

- “Introduction to Statistical Mechanics” by T. Hill (Dover Publications; 1986 edition) - old but a “classic” book;
- “Statistical Mechanics” by D. McQuarrie (University Science Book) - This is an advanced and complete book;
- “Physical Chemistry: Statistical Mechanics” by Horia Metiu (Taylor and Francis, 1st edition) - This is a book for the level of 4th year undergraduate students.

The primary material of the course consists of: references to parallel material in books available in the library, which will be made during the course, your lecture notes, material distributed in the class, examples worked-out on the board and your work on the assignments.

Accessibility

Please contact the course instructor if you require lecture or printed material in an alternate format or if any other arrangements can make this course more accessible to you. You may also wish to contact Services for Students with Disabilities (SSD) at 661-2111 ext. 82147 if you have questions regarding accommodation.

Support Services

Learning-skills counselors at the Student Development Centre (http://www.sdc.uwo.ca) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counseling.

Additional student-run support services are offered by the USC, http://westernusc.ca/services. The website for Registrarial Services is http://www.registrar.uwo.ca.

Students who are in emotional/mental distress should refer to Mental Health@Western http://www.health.uwo.ca/mental_health/ for a complete list of options about how to obtain help.
**Course Evaluation**

**Course Evaluation** 5-6 assignments (20% of the final mark); Mid-term (35%); Final (45% of the final mark).

**Midterm Exam** Two-hour exam, time and place TBA. The format of the exam will be problems and short-answers.

**Final Exam** To be decided by the Registrar’s Office. The final exam will be cumulative, with emphasis on the material that was not examined in the midterm exam. The final will be a three-hour exam and the format of the exam will be problems and short-answers.

To pass the course, you must obtain a minimum of 50% in the average of assignments, midterm and final. One should write the midterm and final exam to pass the course. Obtaining a good average grade in the assignments and midterm is not sufficient to pass the course.

- **Scholastic Offense Policy:** You should be familiar with the Scholastic Offense Policy in the Academic Calendar. Scholastic offenses are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offense, at the following Web site: http://www.uwo.ca/univsec/handbook/appeals/scholastic_discipline_undergrad.pdf.

- **Plagiarism** is a serious Scholastic Offense. Students should write their essays and assignments individually. Copying of assignments will involve penalties in the grades. In essays, whenever a student takes an idea or a passage from another source, appropriate reference should be given.

- **Exam Distress Policy:** It is the policy of the Department of Chemistry that when a student takes a test or an examination, one should have deemed oneself fit to do so. Claims of distress or medical issues after the fact will not be considered as a basis of a grade appeal.

**Absences, Code of Conduct**

- Failure to complete or write the midterm, or the final, or the assignments will result in a mark of zero for the missed item, and potential failure in the course, unless a valid medical or compassionate reason has been approved and an exemption has been granted. The Policy of Accommodation for Medical Illness is found in the web site: https://studentservices.uwo.ca/secure/index.cfm and for further policy information please visit http://www.uwo.ca/univsec/handbook/appeals/accommodation_medical.pdf

- **Missed exam:** If you miss the final exam, contact your Dean’s office to obtain an SPC form. Students who are ill, for all exams and tests yet choose to write the final exam, must accept the mark that they receive.
• **Code of Conduct:** Students are reminded of the University’s Code of Conduct found on the university website. To maintain a high standard of learning environment in our classrooms, those who are disruptive, rude, or show unacceptable behavior, either to the instructor, or the other students, will be asked to leave.

• **Attendance:** Any student who, in the opinion of the instructor, is absent too frequently from class or laboratory periods in any course will be reported to the Dean of the Faculty offering the course (after due warning has been given). On the recommendation of the Department concerned, and with the permission of the Dean of that Faculty, the student will be debarred from taking the regular examination in the course. The Dean of the Faculty offering the course will communicate that decision to the Dean of the Faculty of registration.

**Brief Course Description**

In the course, the basic theory of statistical mechanics with applications will be presented. In the discussion of the applications, relation to molecular simulations will be made. Computations of thermodynamic and structural properties as well as diffusion coefficients will be discussed. The computation of these properties will be applied to ideal gas, Einstein crystal, polyatomic gases, liquids, peptides and other biological systems. The expectation of the course is that the students will understand how the statistical mechanics theory is applied to a variety of problems such as equilibrium constants, phase transitions, physical chemistry of macromolecules, diffusion and molecular simulations.

**Lecture Topics**

**Foundations of Equilibrium Statistical Mechanics**

1. Historical review of statistical mechanics, purpose of statistical mechanics, applications

2. Review of thermodynamics

3. Mathematical tools needed for the course

4. Ensemble average of properties and postulates of statistical mechanics

5. Application of the ensemble theory in the canonical ensemble. Discussion of how to compute mechanical properties (energy, enthalpy, pressure) and thermodynamic properties (entropy, free energy) of matter using appropriate averages over the behaviour of molecules

6. Link of statistical mechanics theory with the molecular simulation methods, Molecular Dynamics and Monte Carlo
7. Fluctuations in statistical mechanics; how to find heat capacities from fluctuations in the energy; equivalence of the ensembles

8. Simplification for the independent molecules and subsystems; Discussion of how to express the partition functions using the quantum and classical description of the microscopic states; Boltzmann statistics

9. Review

Applications of Statistical Mechanics

**Systems of independent molecules**

1. Monoatomic crystals; lattice vibrations; Einstein and Debye models.

2. Ideal monoatomic gas by Boltzmann statistics.

3. Ideal diatomic and polyatomic gases; vibrational, rotational and electronic contributions to thermodynamic functions; chemical equilibria in ideal gases.

**Systems of interacting molecules-Molecular simulations**

1. Pressure

2. Imperfect gases. Second Virial coefficient

3. Applications to liquids. Structure of liquids as described by the radial distribution function. Expression of thermodynamic quantities in terms of the radial distribution function

4. Time correlation functions and Diffusion coefficient

5. Molecular dynamics and Monte Carlo methods
   - integrators
   - force fields
   - periodic boundary conditions
   - treatment of electrostatic interactions
   - temperature and pressure control in the simulations

6. demonstration of how to set up a molecular simulation and how to run it using GROMACS - depending on the knowledge of the students it may be that this part will be replaced with the topic of phase-transitions.
7. Brownian motion and diffusion; Langevin equation for random motions and its application to diffusion and mobility; applications of Langevin dynamics in computations to systems of biological interest

8. Tentative topic: Machine learning in Molecular Simulations

9. Tentative topic: Adsorption of molecules on surfaces

10. Tentative topic: computation of the chemical potential

11. Tentative topic: Debye-Huckel theory and Born model of solvation


13. Tentative topic: the statistical mechanics of the assembly of peptides or nanoparticles or other “soft-matter” problems

14. Review of the material for the final exam

**About the structure of the course**

In the first class, the students and the instructor will discuss certain aspects of the course such as: what applications would the students prefer to discuss in the class? The instructor will provide a number of topics to choose from. Some of the topics in the list may be assigned to the students as reading and assignment.

**Tips to do well in the course**

- Review the material of CHEM2374, CHEM2384, CHEM3374
- keep-up with the course material

**Social Media**

Twitter - Follow us @westernuchem Facebook - www.facebook.com/ChemistryatWestern

**Important dates (2020)**

- Monday, January 6, 2020 - Classes resume
- Tuesday, January 16, 2018 - Last day to add a second-term half course or a second-term full course
- February 15, 2020 - Feb. 23, 2020 - Reading week
- February 17, 2020 - Family day (UWO closed)
• March 7, 2020 - Last day to drop a second-term half course without academic penalty.
• Friday, April 3, 2020 - Classes end