WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 4444B-Statistical Mechanics and Molecular Simulations
January-April 2022

COURSE OUTLINE

Welcome to CHEM 4444B!

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

E-mail sconstas@uwo.ca

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

- January 10 - January 30th, the classes will take place on-line, synchronous mode.
- The in-person classes will take place in ChB 115.
- The mode of course instruction follows the guidelines provided by the University administration.

Office hours 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**.

Brief Course Description

In the course, the basic theory of statistical mechanics with applications mainly in molecular simulations, which are computational statistical mechanics, will be presented. Computations of thermodynamic and structural properties as well as diffusion coefficients will be discussed. The computation of these properties will be applied to polyatomic gases, liquids, solids, and macromolecules . The expectation of the course is that the students will develop a critical understanding of how to assess broadly used simulations methods in a variety of problems in equilibrium constants, (bio)physical chemistry of macromolecules, diffusion, and nano-systems.

Course Learning Outcomes

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

Knowledge of Methods: Obtain problem-solving skills in molecular simulations and (bio)physical chemistry by assignments, on/off-line discussions, use of software, and lecture materials.

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

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

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, simulations.

Autonomy and Professional Capacity: (1) Be able to work productively and collaboratively as a team member. (2) Evaluate the potential impact modelling may have in society, health and environment.

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

- "Physical Chemistry: Statistical Mechanics" by Horia Metiu (Taylor and Francis, 1st edition) - This is a book for the level of 4th year undergraduate students.
- "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 suitable for graduate students in statistical mechanics;
- "Statistical Mechanics: Theory and Molecular Simulation" by M. E. Tuckerman (Oxford University Press, 1st Edition)- Advanced book, suitable for the graduate level.

The primary material of the course consists of: references to parallel material in books available in the library, your lecture notes, examples worked-out in the class, assignments, search of literature for a presentation.

Course Evaluation

Course Evaluation 4 assignments ($4 \times 5\% = 20\%$ of the final mark); one 45-min mid-term exam (15 %); essay written individually (25% of the final mark); oral presentation by

pairs of students (20 %); Final (20 % of the final mark).

Midterm Exam A 45-min in-class midterm exam, on March 2nd. The format of the exam will be problems and short-answers.

- The essay will be discussed with the instructor. It has to be in the field of statistical mechanics or molecular simulations. It will involve a a critically written essay of 7 double-space pages on a textbook topic. References are to be included at the end of the essay. Details will be discussed in the first day of classes.
- The essay should be uploaded in the Dropbox in the owl site of the course by April 8, 2022 at 11:55 pm. The uploaded document should be labeled as "LastName-Essay.pdf". Should you have any questions please contact the instructor directly.

Presentation Oral presentation by pairs of students. Duration of the oral presentation is 15 min (approx. 7.5 min per student). Additional 5 min for questions by the instructor and peers, will be allotted.

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, essay, oral presentation, midterm and final. One should write the midterm and final exam to pass the course. Obtaining a good average grade in the assignments, essay, and presentation is not sufficient to pass the course.
Problem sets will not be accepted for grading after the reports for each activity have been returned and/or the answers discussed with the class or posted on owl. In this class correct answers are posted within 2 weeks of the activity due date. Problem set solutions received 2 weeks after the due activity date will not be graded and that activity will be considered not completed.

Lecture Topics

A selection will be made among the tentative topics in the first day of the class or later. We will be able to cover 2-3 tentative topics.

Foundations of Equilibrium Statistical Mechanics

1. Historical review of statistical mechanics, purpose of statistical mechanics, applications
2. Review of the essentials for the course: thermodynamics and basic quantum mechanics
3. Mathematical methods needed in 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; Boltzmann statistics
9. Review

Applications of Statistical Mechanics

Systems of independent molecules

1. Crystals; lattice vibrations and phonons.
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. Applications to liquids. Structure of liquids as described by the radial distribution function. Expression of thermodynamic quantities in terms of the radial distribution function
2. Time correlation functions and Diffusion coefficient
3. Molecular dynamics and Monte Carlo methods; use of Monte Carlo methods in the simulations of polymers and biological macromolecules
    - integrators
    - force fields
    - periodic boundary conditions
    - treatment of electrostatic interactions
    - temperature and pressure control in the simulations
    - analysis of data

4. demonstration of how to set up a molecular simulation and how to run it using GROMACS; NAMD and comparison of the two softwares.
5. 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
6. Tentative topic: Machine learning in Molecular Simulations
7. Tentative topic: Adsorption of molecules on surfaces
8. Tentative topic: computation of the chemical potential
9. Tentative topic: Debye-Huckel theory and Born model of solvation
10. Tentative topic: Fundamentals of "Soft-Matter"
11. Tentative topic: Sampling of the conformation changes of macromolecules (proteins, nucleic acids)
12. Tentative topic: Solvation models for ions and macroions
13. Tentative topic: Free energy calculation methods
14. Tentative topic: the statistical mechanics of the assembly of peptides or nanoparticles or other "soft-matter" problems
15. Review of the material for the final exam

Assignment dates

- Assignment 1: Release date: January 14; due date January 24
- Assignment 2: Release date: January 26; due date February 7
- Assignment 3: Release date: February 9; due date January 28
- Assignment 4: Release date: March 7; due date March 18

First day 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 above list may be assigned to the students for a presentation.

Accessible Education

- Students with disabilities work with Accessible Education (formerly SSD) which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. The Academic Accommodation for Students with Disabilities policy can be found at:
https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic Accommodation_disabilities.pdf

- 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 Student Accessibility Services (SAS) at (519) 661-2147 if you have any questions regarding accommodations.

Accommodation for Medical Illness or other Serious Circumstances
Students who experience an extenuating circumstance (illness, injury or other extenuating circumstance) sufficiently significant to temporarily render them unable to meet academic requirements may submit a request for academic consideration through the following routes:

(i) Submitting a Self-Reported Absence (SRA) form provided that the conditions for submission are met. To be eligible for a Self-Reported Absence:

- an absence must be no more than 48 hours
- the assessments must be worth no more than 30% of the student's final grade
- no more than two SRAs may be submitted during the Fall/Winter term

(ii) For medical absences, submitting a Student Medical Certificate (SMC) signed by a licensed medical or mental health practitioner to the Academic Counselling office of their Faculty of Registration.

(iii) Submitting appropriate documentation for non-medical absences to the Academic Counselling office in their Faculty of Registration. Note that in all cases, students are required to contact their instructors within 24 hours of the end of the period covered, unless otherwise instructed in the course outline. For further information, please consult the university's policy on academic consideration for student absences:
https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_ Consideration_for_absences.pdf.

Students should also note that individual instructors are not permitted to receive documentation directly from a student, whether in support of an application for consideration on medical grounds, or for other reasons. All documentation required for absences that are not covered by the Self-Reported Absence Policy must be submitted to the Academic Counselling office of a student's Home Faculty.

Religious Accommodation

Students should consult the University's list of recognized religious holidays, and should give reasonable notice in writing, prior to the holiday, to the Instructor and an Academic Counsellor if their course requirements will be affected by a religious observance. Additional information is given in the Western Multicultural Calendar:
https://multiculturalcalendar.com/ecal/index.php?s=c-univwo

Make-up exams
If a student misses a midterm exam, a make-up exam may be provided upon a recommendation from academic counseling. If the make-up date is still not met because of a valid reason, then the weighting of the miss exam, will be redistributed to other evaluation components. For example, if you miss the Midterm the weight will be transferred to the final exam. If you miss the final exam for a valid reason, a "Recommendation of Special Examination" form must be obtained from the Dean's Office. A designated date for the special exam will be provided later in the term by the Dean's office.

Academic Policies

The website for Registrarial Services is http://www.registrar.uwo.ca.
E-mailing: In accordance with policy,
http://www.uwo.ca/its/identity/activatenonstudent.html,
the centrally administered e-mail account provided to students will be considered the individual's official university e-mail address. It is the responsibility of the account holder to ensure that e- mail sent by the University to his/her/their official university address is attended to in a timely manner.
Electronic devices: electronic devices will or will not be permitted on tests and exams. Only a non-programmable calculator can be used in midterms and final exam.
Scholastic offences: Scholastic offences, including plagiarism, are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site:
http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf.
All required papers may be subject to submission for textual similarity review to the commercial plagiarism detection software under license to the University for the detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between The University of Western Ontario and Turnitin.com (http://www.turnitin.com).
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.

Support Services

Academic matters: Please visit the Science & Basic Medical Sciences Academic Counselling webpage for information on add/drop courses, academic considerations for absences, appeals, exam conflicts, and many other academic related matters:
https://www.uwo.ca/sci/counselling/

Managing academics and well-being: Western University is committed to a thriving campus as we deliver our courses in the mixed model of both virtual and face-to-face formats. We encourage you to check out the Digital Student Experience website to manage your academics and well- being: https://www.uwo.ca/se/digital/.

Learning-skills Services: Learning-skills counsellors 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 counselling.

Emotional/mental distress services: Students who are in emotional/mental distress should refer to Mental Health Western (https://www.uwo.ca/health/psych/index.html) for a complete list of options about how to obtain help. Other services: Additional student-run support services are offered by the USC, https://westernusc.ca/your-services/#studentservices

Social Media

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

Important dates (2022)

- January 4 University re-opens
- January 10 Classes resume (online)
- January 18 Deadline to add a second-term course
- January 31 Planned return to in-person instruction
- Feb. 19–27 Reading Week
- March 14 Deadline to drop a second-term course without academic penalty
- April 8 Last day of classes
- April 9 Study Day

- April 10–30 Final Exams (excluding April 15–17 for Easter and Passover)