WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 9444B-Statistical Mechanics and Molecular Simulations
January-April 2022

Welcome to CHEM 9444B!

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

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

Office hours By appointment

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

Brief Course Description

In the course, the basic theory of statistical mechanics with applications will be presented. The applications will be mainly in molecular simulations. 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, (bio)physical chemistry of macromolecules, diffusion and molecular simulations.

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 Material

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.
Helpful optional 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.

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.

Course Evaluation

- 4 Assignments: $4 \times 5\% = 20\%$ of the final mark.
- Midterm Exam: 15% of the final mark. A 45-min in-class midterm exam, date TBA. The format of the exam will be problems and short-answers.
- Project: 45 % of the final mark = 20% 15 min oral presentation in-pairs with other graduate students and 25% essay - individual. In the event that the student is unpaired the oral presentation will be individual.
  - The project 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 10 double-space pages and an oral presentation.
  - The essay should explain in-depth the topic of your choice. It can be based on one article but you can use many articles in order to understand the article or topic of your choice. List of references should be provided at the end of the essay. The essay should not be a simple statement of facts that one reads in an article, but it should have a critical assessment of the article (i.e. you should address "why" and "how").
  - The essay should be uploaded in the Dropbox in the owl site of the course by March 30, 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.
- Final Take-home Exam: 20% of the final grade. 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. The exam may contain additional or different problems from those that will test the undergraduate students.

To pass the course, you must obtain a minimum of 50% in the average of assignments, oral presentation, essay, 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.

Lecture Topics

Foundations of Equilibrium Statistical Mechanics

1. Historical review of statistical mechanics, purpose of statistical mechanics, applications
2. Review of thermodynamics
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; 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 and Molecular Simulations

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. Molecular dynamics and Monte Carlo methods
    - integrators
    - force fields
    - periodic boundary conditions
    - treatment of electrostatic interactions
    - temperature and pressure control in the simulations
    - analysis of data; Radial distribution functions
5. demonstration of how to set up a molecular simulation and how to run it using GROMACS
6. 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
7. Tentative topic: Machine learning in Molecular Simulations
8. Tentative topic: Adsorption of molecules on surfaces
9. Tentative topic: computation of the chemical potential
10. Tentative topic: Debye-Huckel theory and Born model of solvation

11. Tentative topic: Fundamentals of "Soft-Matter"
12. Tentative topic: Sampling of the conformation changes of macromolecules (proteins, nucleic acids)
13. Tentative topic: Solvation models for ions and macroions
14. Tentative topic: Free energy calculation methods
15. Tentative topic: the statistical mechanics of the assembly of peptides or nanoparticles or other "soft-matter" problems
16. Review of the material for the final exam

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 for a presentation.

Policies and Accommodation

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.

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.

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

Course attendance and missed/late assignments

If you are unable to meet a course requirement due to illness or other serious circumstances, you must provide valid medical or other supporting documentation to your instructor immediately. It is the student's responsibility to make alternative arrangements with their instructor once the accommodation has been approved and the instructor has been informed.

Notes on Academic Honesty

Scholastic offences 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:
www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_grad.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 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).

Health and Wellness

As part of a successful graduate student experience at Western, we encourage students to make their health and wellness a priority. Western provides several on campus health-related services to help you achieve optimum health and engage in healthy living while pursuing your graduate degree. For example, to support physical activity, all students, as part of their registration, receive membership in Western's Campus Recreation Centre. Numerous cultural events are offered throughout the year. For example, please check out the Faculty of Music web page http://www.music.uwo.ca/, and our own McIntosh Gallery http://www.mcintoshgallery.ca/.

Information regarding health- and wellness-related services available to students may be found at http://www.health.uwo.ca/. Students seeking help regarding mental health concerns are advised to speak to someone they feel comfortable confiding in, such as their faculty supervisor, their program director (graduate chair), or other relevant administrators in their unit. Campus mental health resources may be found at http://www.health.uwo.ca/mental_health/resources.html.

Other Support 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 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.

Tips to study for the course

- Review material on probabilities.
- Review the material of CHEM2374 (2nd year Thermodynamics), CHEM2384, CHEM3374 if you are from Western, or review the undergraduate material on thermodynamics, statistical mechanics, basic quantum mechanics.
- Do the assignments gradually as the material progresses.
- Keep-up with the course material, discuss questions with peers in the class and in the owl forum.
- Participate in the class by answering questions and by asking questions.

Social Media

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

Important dates

- Monday, January 3 - Classes resume
- Tuesday, January 11 - Last day to add a second-term half course or a second-term full course
- February 19 - Feb. 27 - Reading week
- February 21 - Family day (UWO closed)
- March 7 - Last day to drop a second-term half course without academic penalty.
- Friday, April 1, 2022 - Classes end