WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 9654Q-Advanced Methods in Molecular Simulations
October-December 2018

COURSE OUTLINE

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

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Lecture times  Wed. 3:00 - 4:00 pm and Friday 2:30 - 4:30 pm.

Location  TBA

Office hours  Any time by appointment

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

Prerequisites:  CHEM2374A (Thermodynamics) and CHEM2384B (Microscopic phenomena) or the course analogues for students who have not taken their courses at Western. CHEM4444 (Statistical Mechanics and Molecular and Molecular Simulations) is a very helpful background to have but if missing, the student may catch up with additional reading. CHEM 9654Q will assume knowledge in electrostatics that may have been learned in CHEM 9554Q or in physics or other Departments. Knowledge of MATLAB, MAPLE or Mathematica will be very helpful for the assignments.

Course Learning Outcomes

Breadth and Depth of Knowledge:  Be able to describe the fundamental scientific principles of simulations and electrostatics and apply these principles in chemical systems 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 assignments and essay.

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, essay.

Autonomy and Professional Capacity:  (1) Be able to work productively and collaboratively as a team member. (2) Communicate the results by preparing and presenting an essay.
Accessibility

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

Material

Material presented in the class and assigned reading. Suggested textbooks:

- “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.
- “Understanding Molecular Simulation: From Algorithms to Application” by D. Frenkel and B. Smit
- “Introduction to Electrodynamics” by David J. Griffiths, 4th Edition;
- A classic advanced book in electrostatics and electrodynamics is: “Classical Electrodynamics” by John David Jackson, 3rd Edition or higher.

Moreover, the instructor will suggest acceptable websites which provide high level of material.

The students have to keep lecture notes based on the discussion in the class and the blackboard writing.

Course Evaluation 3 assignments (30 % of the final mark); A take-home midterm exam (20 % of the final mark) and a project (50 % of the final mark).

Project The project will be discussed with the instructor. It will involve an essay of 10 double-space pages and a 30 min class presentation with questions asked by the instructor and audience (20 min presentation + 10 min of questions). The essay and oral presentation worth, 25 % and 25 %, respectively.
To pass the course, you must obtain a minimum of 50% in the average of assignments, midterm and project. Obtaining a good average grade in the assignments and midterm is not sufficient to pass the course.

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

- **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 Deans 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 the class 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**

The course will discuss advanced simulation methods with applications in chemical and biochemical systems.

**Tentative Lecture Topics**

1. Liouville equation (≈ 1 hour)
2. Advanced molecular Dynamics algorithms (≈ 3 hours)
3. Advanced Monte Carlo algorithms (≈ 2 hours)
4. Rare event dynamics (≈ 2 hours)
5. Replica Exchange Molecular Dynamics and other replica based algorithms (≈ 2 hours)
6. Free energy calculation methods - Alchemical transformations (≈ 4 hours)
7. Soft matter simulations - colloids, forces among colloidal particles (≈ 3 hours)

**Social Media**

Twitter - Follow us @westernuchem
Facebook - www.facebook.com/ChemistryatWestern
Important dates (2018)

September 6: Classes start
October 8: Thanksgiving Holiday
October 9 – October 12: Fall Reading Week
Midterm date: November 15
November 12: Last day to drop a first-term half course or a first-term full course (2018-19 Fall/Winter Term) without academic penalty
December 7: Fall Term classes end
Final exam date will be determined by the registrar’s office
January 7, 2019: Classes resume