WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 9484T-Electrostatics of Chemical Systems
Quarter Graduate Course 2024

COURSE OUTLINE

Office hours By appointment

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

Brief Course Description

The basic theory of electrostatics will be discussed with applications into chemical and biochemical problems. Chemical problems that will be discussed are polarizability, intermolecular forces, usage of electrostatics in molecular simulations. In biological systems, the role of electrostatics in the stability and charging of proteins and nucleic acids will be discussed. Applications will be performed by using computational software such as NAMD.

Course Learning Outcomes

Breadth and Depth of Knowledge: Be able to describe the fundamental principles of electrostatics and apply these principles in chemical and biochemical systems such as solutions, stability of proteins and nucleic acids.
Application of Knowledge: Be able to apply the knowledge to predict and rationalize the physical and chemical properties of chemical and biochemical systems and to critically use computer simulation methods.
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 computational results by training on case studies, lectures, assignments, essay.
Autonomy and Professional Capacity: (i) Be able to work productively and collaboratively individually and as a team member. (ii) Communicate the results to peers and instructor 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:

1. "Computer Simulation of Liquids" by M. P. Allen and D. J. Tildesley, 3rd Edition.
2. "Introduction to Electrodynamics" by David J. Griffiths, 4th Edition;
3. "Classical Electrodynamics" by John David Jackson, 3rd Edition or higher.

Course Evaluation 3 assignments (30 % of the final mark); Midterm (35 %); Project (35 % of the final mark).

Midterm Exam Two-hour exam. The format of the exam will be problems and short-answers.

Project The project, can be of computational or of theoretical nature, it will be discussed with the instructor. It will involve an essay of 10 double-space pages and a 16 min ($\pm$ 1 min) class presentation with questions asked by the instructor and audience. The essay and oral presentation worth, 20 % and 15 %, 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. The student should write the midterm and prepare the project to pass the course.

Tentative Lecture Topics

1. Basics of electrostatics that apply in chemistry and biochemistry: Coulomb's law, electric field, potential, Gauss's law, energy of electrostatic systems, self-energy, Laplace equation, Poisson equation, boundary conditions and solutions. Numerical solution of Poisson equation. Introduction to MAPLE for solving electrostatic problems ($\approx$ 3 hours)
2. Multipole expansion with application to intermolecular forces ($\approx$ 1 hour)
3. Ion and macroion-solvent interactions from atomistic modelling ($\approx$ 1 hour)
4. Poisson-Boltzmann equation for proteins and other macromolecules; solutions under different boundary conditions; numerical solution using MAPLE and NAMD; Debye-Huckel theory; ionic strength of solutions; models for electrolytes ($\approx$ 3 hours)
5. Implicit solvation; Born solvation energy ($\approx$ 1 hour)
6. Electric double layer ($\approx$ 1 hour)

7. Treatment of electrostatic interactions in molecular simulations. Ewald summation, reaction field methods, multi-level summation; Subtleties in the method implementation. Use of the software NAMD to perform computational tests ($\approx$ 2 hours)

8. Polarizability and polarizable molecular models used in simulations ($\approx$ 2 hours)

9. Proton and electron transfer processes ($\approx$ 2 hours)

10. Polyelectrolytes; Charging of proteins in gaseous phase and solutions ($\approx$ 1 hour)

11. Charge-induced instabilities in proteins - Rayleigh model for macromolecules ($\approx$ 1 hour)

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 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 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.

Social Media

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