CHEM 4444a: Computer Simulations in Chemistry

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Computer Simulations in Chemistry

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Lecture times Monday, Tuesday, Thursday, 12:30-1:30 pm, Room 115-Chemistry Building

Office hours Monday, Tuesday, Thursday 11:30-12:30 pm or by appointment

Website http://instruct.uwo.ca/chemistry/4444a
In the website notes of the course will be posted.

Textbook

"Physical Chemistry: Statistical Mechanics" by Horia Metiu. This textbook can be found in the University Bookstore. (optional) Other useful books are any of the following:

- "Introduction to Statistical Mechanics" by T. Hill;
- "Statistical Mechanics" by D. McQuarrie;
- "Molecular Dynamics Simulation, Elementary Methods" by J.M. Haile.

All books are on reserve in the library. They can also be found in the University bookstore. The primary material of the course consists of: references to parallel material in various books available in the library which will be made during the course, your lecture notes, material distributed in the class and your work on the assignments.

General description

Methods of Molecular Dynamics and Monte Carlo based on the theory of Statistical Mechanics can be used to study equilibrium properties in all states of matter. In the course, the basic theory of statistical mechanics will be presented with applications in computer simulations. The objective of the course is to develop to the students a critical understanding of the simulation techniques. This goal will be achieved by presenting both the basic theory of statistical mechanics as well as the algorithms involved in the simulations. The expectation of the course is that the students will be able to use simulation codes with the understanding of the methods and control the simulations.

Course evaluation

Course Evaluation 6-7 assignments (20 % of the final mark); Mid-term (35 %); Final (45 % of the final mark).

Midterm Exam Two hour exam. Approximately one day between October 19 to October 23rd, 2009.

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.

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 CHEM 3374A/B, CHEM 3384F/G or the former Chemistry 354 a/b. Antirequisites are the former Chemistry 464a/b.

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
- 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.
- We will not authorize SPC exams for students with three exams in 27 (or greater) hours, nor for those with exam conflicts. The Registrar will place those with conflicts in designated conflict rooms. However, we will be pleased to approve your SPC if you have a three in 24.
- Students are reminded of the universitys 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.

Foundations of Molecular Simulations and Equilibrium Statistical Mechanics

1. Use of computer simulations. Role of statistical mechanics.
2. Objectives of statistical mechanics. Review of thermodynamics.
3. Ensemble average of properties and postulates of statistical mechanics.
4. Application of the ensemble theory on 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.

Foundations of Molecular Simulations and Equilibrium Statistical Mechanics

1. Fluctuations in statistical mechanics; how to find heat capacities from fluctuations in the energy; equivalence of the ensembles.
2. Simplification for the independent molecules and subsystems; Discussion of how to express partition functions using the quantum and classical description of the microscopic states; Boltzmann statistics.

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.

Applications of Statistical Mechanics

Systems of interacting molecules-Computer simulations

1. Intermolecular Forces and Molecular Mechanics.
2. Molecular Dynamics and Basic Algorithms.
3. Running Simulations. How a simulation is set up.
4. Instruction of how to use GROMACS. This can be done in your laptop or in a computer in my lab. The students have the option to write their own molecular dynamics code for a small system and use it to compute properties.
5. Periodic boundary conditions used for simulations of bulk systems.

Applications of Statistical Mechanics

Systems of interacting molecules-Computer simulations

1. Applications to liquids. Structure of liquids as described by the radial distribution function.
2. Computation of diffusion coefficients.
3. Monte Carlo schemes and algorithms.
4. Models for polymer systems for the study of equilibrium properties.
5. Imperfect gases. Second Virial coefficient.

Chemical reaction rates and diffusion

1. Activated complex theory (transition state theory) of the rate of bimolecular gas phase reactions. Femtochemistry.
2. Chemical kinetics in solution; influence of solvent; transition state theory and recrossing corrections.
3. Brownian motion and diffusion; Langevin equation for random motions and its application to diffusion and mobility.