CHEM 864

Statistical Mechanics

Spring 2024

Instructor:

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Lectures and Group Projects:

MWF 11:00am–11:50am, Room 7421, North Tower, Chemistry Building

Course Website:

https://canvas.wisc.edu/courses/381411

COURSE DESCRIPTION

This course is focused on classical statistical mechanics and its applications in condensed phases. In this course, we will first review the fundamental principles of statistical mechanics theories. We will then delve into kinetic theories and explore their applications ranging from chemical reactions to protein conformational changes. Building upon these theories, we will teach students a variety of molecular simulation tools and advanced algorithms to investigate dynamics of chemical and biological systems. Finally, we will encompass statistical mechanics theories relevant to the thermodynamic and structural properties of the condensed liquid phases, including theories underlying advanced enhanced sampling techniques. Through a series of group projects, students will also gain hands-on experience with various simulation tools and machine learning algorithms. Additionally, they will have the opportunity to develop their coding skills to compute thermodynamic and kinetic properties of chemical and biological systems.

COURSE LEARNING OUTCOMES

After completing this course, students are expected to:

- Understand statistical mechanics theories pertaining to the kinetics of chemical and biological systems in condensed phases.
- Grasp statistical mechanics theories related to the thermodynamic and structural properties of condensed liquid phases.
- Acquire hands-on experience with a variety of molecular simulation tools.
- Cultivate coding skills for the analysis of simulation data.

MEETING TIME & LOCATION

- **Unit 1** (review of basic theories) - **Lectures:** Mon, Wed, Fri, 11:00–11:50am, Room 7421
- **Unit 2** (kinetics) & **Unit 3** (thermodynamics)

  - **Lectures**, Mo, Wed, 11:00–11:50am, Room 7421

  - Group projects, Fri, 11:00–11:50am, Room 7421

RECOMMENDED TEXTBOOKS

There is no required textbook for this course. However, we highly recommend students to read the following books to gain a deeper understanding of the subjects introduced in class.

- "An introduction to statistical thermodynamic" by Terrell L. Hill, Dover Publications, INC, New York, 1986.
- "Statistical Mechanics" by Donald Allan McQuarrie, University Science Books, 2000
- "Introduction to modern statistical mechanics" by David Chandler, New York: Oxford University Press, 1987.
- "Computer Simulation of Liquids" by M.P. Allen and D.J. Tildesley, Oxford Science Publications

STUDENT REQUIREMENT

- Students need to be familiar with the syllabus and the class schedule, and be aware of the course requirements and progress.
- Students need to check the course website (https://canvas.wisc.edu/courses/381411) and their WISC e-mail on regular basis. The slides and other course materials will be posted on the course website. Furthermore, course announcements will also be made on the course website and/or via e-mail.
- Students' Rules, Rights & Responsibilities: Students can refer to the following link for the university's privacy rights (FERPA): https://guide.wisc.edu/undergraduate/#rulesrightsandresponsibilitiestext
- Additional information regarding UW-Madison's academic policies including academic integrity is available at the end of the Course Syllabus.

CREDITS: 3 credits. The credit standard for this course is met by an expectation of a total of 135 hours (3-credit) of student engagement with the course learning activities (at least 45 hours per credit), which include regularly scheduled lectures, instructor-student meeting times, reading, writing, group projects, and other student work as described in the syllabus.

REGULAR & SUBSTANTIVE INTERACTIONS:

- Participation in classes where there is an opportunity for direct interaction between the student and the instructor.
- Provide personalized comments or discussions with students on their group projects.
- Post announcements and email about academic aspects of the class.
- Use of small groups that are moderated by the instructor to discuss the simulation software

tool and final projects.

REQUISITES: Graduate/professional standing

COURSE DESIGNATION:

- Grad 50% - Counts toward 50% graduate coursework requirement

INSTRUCTIONAL MODALITY: In-person

GRADING

The grade is determined by the following two tasks: group projects and an open-book final exam.

1. **Group projects (4*15% = 60%)**: Students will be divided into groups (mostly 2 students per group) to complete the group projects. There are 4 group projects, and each contributes to 15% of the total grades. For the assessments of group projects, each group will submit their codes/scripts and give short presentations to the instruction team.
2. **Final exam (40%)**: We will conduct an in-class and **open-book** final exam.

COURSE SCHEDULE (Updated on Jan 22, 2024)

Unit 1: Statistical Thermodynamics Theories		
Week 1	Jan 24, Wed	**Lecture:** Introduction & Group Assignments
	Jan 26, Fri	**Lecture:** Chapter 1: Statistical Thermodynamics Fundamentals (Boltzmann distribution, ensembles, partition functions, and fluctuations.)
Week 2	Jan 29, Mon	**Lecture:** Chapter 1: Statistical Thermodynamics Fundamentals
	Jan 31, Wed	**Lecture:** Chapter 1: Statistical Thermodynamics Fundamentals
	Feb 2, Fri	**Lecture:** Chapter 1: Statistical Thermodynamics Fundamentals
Week 3	Feb 5, Mon	**Lecture**: Chapter 2: Applications to Simple Systems (Independent molecules, ideal gas, and monoatomic crystals.)
	Feb 7, Wed	**Lecture**: Chapter 2: Applications to Simple Systems
	Feb 9, Fri	**Lecture**: Chapter 2: Applications to Simple Systems
Week 4	Feb 12, Mon	**Lecture**: Chapter 2: Applications to Simple Systems
	Feb 14, Wed	**Lecture**: Chapter 2: Applications to Simple Systems
	Feb 16, Fri	**Lecture**: Chapter 2: Applications to Simple Systems
Unit 2: Kinetic Theories: From Chemical Reactions to Protein Conformational Changes		
Week 5	Feb 19, Mon	**Lecture:** Chapter 3: Rate Theories (Transition state theory, Kramer's theory, Langevin equation, fluctuation-dissipation, diffusion)

	Feb 21, Wed	**Lecture:** Chapter 3: Rate Theories
	Feb 23, Fri	**Group Project 1:** MD simulations and calculations of kinetic properties
Week 6	Feb 26, Mon	**Lecture:** Chapter 3: Rate Theories
	Feb 28, Wed	**Lecture:** Chapter 3: Rate Theories
	Mar 1, Fri	**Group Project 1:** MD simulations and calculations of kinetic properties
Week 7	Mar 4, Mon	**Lecture:** Chapter 4: Molecular Dynamics Simulations
	Mar 6, Wed	**Lecture:** Chapter 4: Molecular Dynamics Simulations
	Mar 8, Fri	**Group Project 2:** Kinetic analysis of Alanine Dipeptide simulation datasets using VAMPnets and MSMs.
Week 8	Mar 11, Mon	**Lecture:** Chapter 4: Molecular Dynamics Simulations
	Mar 13, Wed	**Lecture:** Chapter 5: Protein Dynamics
	Mar 15, Fri	**Group Project 2:** Kinetic analysis of Alanine Dipeptide simulation datasets using VAMPnets and MSMs.
Week 9	Mar 18, Mon	**Lecture:** Chapter 5: Protein Dynamics
	Mar 20, Wed	**Lecture:** Chapter 5: Protein Dynamics
	Mar 22, Fri	**Group Project 2:** Kinetic analysis of Alanine Dipeptide simulation datasets using VAMPnets and MSMs.
Week 10	Mar 25-29	**Spring Recess**
Unit 3: Thermodynamic and Structural Properties in the Condensed Phase		
Week 11	Apr 1, Mon	**Lecture:** Chapter 6: Free Energy Calculations
	Apr 3, Wed	**Lecture:** Chapter 6: Free Energy Calculations
	Apr 5, Fri	**Group Project 3:** Calculations of Potential of Mean Force for Methane Dimerization in Water via Umbrella Sampling
Week 12	Apr 8, Mon	**Lecture:** Chapter 6: Free Energy Calculations
	Apr 10, Wed	**Lecture:** Chapter 7: Liquid Structure (Distribution functions, simple liquid theories, and Debye-Hückel theory)
	Apr 12, Fri	**Group Project 3:** Calculations of Potential of Mean Force for Methane Dimerization in Water via Umbrella Sampling
Week 13	Apr 15, Mon	**Lecture:** Chapter 7: Liquid Structure
	Apr 17, Wed	**Lecture:** Chapter 7: Liquid Structure
	Apr 19, Fri	**Group Project 4:** Replica Exchange Molecular Dynamics Simulations
Week 14	Apr 22, Mon	**Lecture:** Chapter 8: Expanded Ensembles and Enhanced

		Sampling Techniques
	Apr 24, Wed	**Lecture:** Chapter 8: Expanded Ensembles and Enhanced Sampling Techniques
	Apr 26, Fri	**Group Project 4:** Replica Exchange Molecular Dynamics Simulations
Week 15	Apr 29, Mon	**Lecture:** Chapter 8: Expanded Ensembles and Enhanced Sampling Techniques
	May 1, Wed	Review
	May 3, Fri	**Final exam**

DIVERSITY & INCLUSION STATEMENT

Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals. The University of Wisconsin-Madison fulfills its public mission by creating a welcoming and inclusive community for people from every background – people who as students, faculty, and staff serve Wisconsin and the world.

ACADEMIC INTEGRITY STATEMENT

By virtue of enrollment, each student agrees to uphold the high academic standards of the University of Wisconsin-Madison; academic misconduct is behavior that negatively impacts the integrity of the institution. Cheating, fabrication, plagiarism, unauthorized collaboration, and helping others commit these previously listed acts are examples of misconduct which may result in disciplinary action. Examples of disciplinary action include, but is not limited to, failure on the assignment/course, written reprimand, disciplinary probation, suspension, or expulsion.

ACCOMMODATIONS FOR STUDENTS WITH DISABILITIES STATEMENTS

The University of Wisconsin-Madison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform faculty [me] of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. Faculty [I], will work either directly with the student [you] or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA. (See: McBurney Disability Resource Center)

ACADEMIC CALENDAR & RELIGIOUS OBSERVANCES

Students can refer to the following link for the current and future academic calendars, along with the university's religious observance policy: https://secfac.wisc.edu/academic-calendar/