

Chemistry 435: Survey of Modern Physical Chemistry (Fall 2023)
Department of Chemistry & Biochemistry, Loyola University Chicago

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Please use CHEM435 in the email subject
- Office Hours:** Thursdays 2:30-3:30pm (Dr. Li, Weeks 1-6) or by appointment
By appointment (Dr. Killelea, Weeks 7-15)
- Class:** Tuesdays & Thursdays, 6:00-7:15 pm, Flanner Hall 105
- Course Prerequisites:** Graduate standing.
- Require Materials:** A calculator capable of scientific notation.
- Supplementary Texts:** *Quantum Mechanics: Atkins' Physical Chemistry*, Atkins, Paula, and Keeler (11th edition), *Quantum Chemistry*, Donald A. McQuarrie; *Statistical Thermodynamics: Statistical Mechanics*, Donald A. McQuarrie.

Course Overview

This course is comprised of a review of quantum mechanics and statistical thermodynamics. Quantum mechanics is the best model we presently have available for describing the behavior of microscopic (e.g. atomic scale) systems. Developed in the early 1900's, the theory has been essential for understanding many of the scientific advances in the past hundred years and has enabled a sometimes clear picture of atomic-scale phenomena. A qualitative understanding of quantum is necessary for a chemist, and an understanding of the fundamentals of quantum mechanics is valuable for any chemistry involved with research. Many 'ordinary' techniques in chemistry, for example, absorption of light (spectroscopy), the structure of solids, and semiconductor devices, are all so-called 'quantum' phenomena. A key goal will be to de-mystify many of the 'odd' behaviors that have been casually assigned to quantum mechanics. Quantum mechanics also allows for the calculation of molecular energy states, and statistical mechanics is the modern approach to bridge the gap between atomic-scale phenomena and macroscopic observations. We will superficially review some of the key components of statistical thermodynamics, largely focused on entropy.

Class Preparation: In order to understand the material presented during lectures, it is important to come to the class with good background knowledge. This can be achieved by reading (and thinking about) material in the supplementary textbook, reviewing appropriate material from calculus, physics, and general chemistry classes. Work together with your classmates; if you don't understand something, someone else may. You will also find that explaining a solution to your classmate will improve your understanding and long-term retention of the material. I cannot overstate how much more useful the classes will be if you come into the room well prepared, and even better, with questions for us and your fellow classmates. The three keys to success in physical chemistry are reading the text, solving as many problems as possible, and asking questions! Ask us questions about the material in class and office hours and ask your classmates questions. It is recommended that students devote to the preparation for this class a minimum of one hour every day.

Exams, Homework, and Grading

There will be three exams this semester, each corresponding to the topical split (first two for quantum and the last one for stat mech). Details regarding these evaluations will be forthcoming.

Final Exam: It is presently not planned to have a final exam. However, this may change, and the final exam time is Tuesday, 12 Dec 2023 at 7:00pm in FH-105.

Homework: You will have homework assignments to complement the materials covered in the class. The homework assignments will be graded for completeness. You will have 5 days to finish each homework assignment. Due date may be postponed for excused absences that last three or more days. Late homework turned in within 72 hours of the due time will receive 50% of the credits, while late homework turned in after 72 hours of the due time will receive zero points.

Grading: The grade will be based on the exams, seminar, and homework assignments.

400 Points Total

Exam 1:	100	points
Exam 2:	100	points
Exam 3:	100	points
Seminar:	50	points
Homeworks:	50	points
Course Evaluation:	5	bonus points
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	405	points

Midterm Grade: Your midterm grades will be obtained based on Exam 1 (100 points), Seminar (50 points) and homework assignments (50 points) according to the method described below.

Grading Scale (400 points in total):

≥ 90%	A
85-90	A-
80-85	B+
75-80	B
70-75	B-
65-70	C+
60-65	C
55-60	C-
40-55	D
< 40	F

Tentative Schedule

Note: The instructors reserve the right to make changes to the schedule, and to move things around. This is simply an outline.

<i>Date</i>	<i>Class</i>	<i>Topics</i>	<i>Readings</i>	<i>other</i>
29 Aug	1	Origins of quantum mechanics	Topic 7A of Atkins' Physical Chemistry (11 th edition)	
31 Aug	2	Wave mechanics: Wavefunctions, operators and observables	Topic 7B, 7C	
5 Sep	3	Translational motion	Topic 7D	
7 Sep	4	Vibrational motion	Topic 7E	
12 Sep	5	Rotational motion	Topic 7F	
14 Sep	6	Hydrogenic atoms	Topic 8A	
19 Sep	7	Many-electron atoms	Topic 8B	
21 Sep	8	Valence-bond theory	Topic 9A	
26 Sep	9	Molecular orbital theory	Topic 9B	
28 Sep	10	Molecular orbital theory: diatomic molecules & polyatomic molecules	Topics 9C, 9D, 9E	
3 Oct	11	Seminar		
5 Oct	12	Exam 1 (take home)		
10 Oct	Fall Break NO CLASS			
12 Oct	13	Classical wave equation	Handout	
17 Oct	14			
19 Oct	15	Review of Schrödinger equation	McQuarrie, Quantum Chem., Ch. 3	
24 Oct	16			
26 Oct	17	Review of quantum mechanics	McQuarrie, Quantum Chem., Ch. 4	
31 Oct	18			
2 Nov	19	Exam 2 (take home)		
7 Nov	20	Intro to statistical mechanics	McQuarrie, Stat .Mech., Ch. 1	
9 Nov	21			
14 Nov	22	Canonical ensemble	Ch. 2	
16 Nov	23			
21 Nov	24	Other ensembles	Ch. 3	
23 Nov	Thanksgiving Break NO CLASS			
28 Nov	25	Statistics	Ch. 4	
30 Nov	26			
5 Dec	27	Ideal Gas	Ch. 5	
7 Dec	28	Exam 3 (take home)		

Pass/Fail Conversion Deadlines and Audit Policy

A student may request to convert a course into or out of the “Pass/No-Pass” or “Audit” status only within the first two weeks of the semester. For the Fall 2023 semester, students can convert a class to “Pass/No-Pass” or “Audit” through Monday, September 11th. Students must submit a request for Pass/No-Pass or Audit to their Academic Advisor.

Health, Safety, and Well-Being On-Campus

Please be familiar with and adhere to all guidelines posted on the *Health, Safety, and Well-Being Update* site: (<https://www.luc.edu/healthsafetyandwellbeing/>.) This site relays important updates and protocols related to COVID-19 and other matters.

Final Exam

The University sets the schedule for all final exams. The final will be held on:

Tuesday 12 Dec 2023 at 7:00pm (CST)

You will have exactly 2 hours to complete the exam. Additional time will not be granted, even if you start late. There will be no make-up final exams given under any circumstance, and the exam will not be given early, either.

Instructors may not reschedule final exams for a class for another day and/or time during the final exam period. There can be no divergence from the posted schedule of dates for final exams. Individual students who have four (4) final examinations scheduled for the same date may request to have one of those exams rescheduled. If a student reports having four final examinations scheduled for the same date, students should be directed to e-mail a petition to Adam Patricoski, Assistant Dean for Student Academic Affairs, CAS Dean’s Office (apatricoski@luc.edu).

Course Repeat Rule

Effective with the Fall 2017 semester, students are allowed only THREE attempts to pass Chemistry courses with a C- or better grade. The three attempts include withdrawals (W). The Department advises that it is preferable to complete a course with a grade of C or C-, and to demonstrate growth in future coursework, than to withdraw from a course.

After the second attempt, the student must secure approval for a third attempt. Students must come to the Chemistry Department, fill out a permission to register form or print it from the Department of Chemistry & Biochemistry website: <https://www.luc.edu/chemistry/forms/> and personally meet and obtain a signature from either the Undergraduate Program Director, Assistant Chairperson, or Chairperson in Chemistry. A copy of this form is then taken to your Academic Advisor in Sullivan to secure final permission for the attempt.

Student Accommodations

Loyola University Chicago provides reasonable accommodations for students with disabilities. Any student requesting accommodations related to a disability or other condition is required to register with the Student Accessibility Center (SAC). Professors will receive an accommodation notification from SAC, preferably within the first two weeks of class. Students are encouraged to meet with their professor individually in order to discuss their accommodations. All information will remain confidential. Please note that in this class, software may be used to audio record class lectures in order to provide equitable access to students with disabilities. Students approved for this accommodation use recordings for their personal study only

and recordings may not be shared with other people or used in any way against the faculty member, other lecturers, or students whose classroom comments are recorded as part of the class activity. Recordings are deleted at the end of the semester. For more information about registering with SAC or questions about accommodations, please contact SAC at 773-508-3700 or SAC@luc.edu.

Academic Integrity

All students in this course are expected to have read and to abide by the demanding standard of personal honesty, drafted by the College of Arts & Sciences, which can be viewed at:

<https://www.luc.edu/cas/advising/academicintegritystatement/>

A basic mission of a university is to search for and to communicate the truth as it is honestly perceived. A genuine learning community cannot exist unless this demanding standard is a fundamental tenet of the intellectual life of the community. Students of Loyola University Chicago are expected to know, to respect, and to practice this standard of personal honesty.

Academic dishonesty can take several forms, including, but not limited to cheating, plagiarism, copying another student's work, submitting false documents, and deliberately disrupting the performance of other class members. Standards apply to both individual and group assignments.

Regarding the use of Artificial Intelligence: our Provost has expressed to “Let us all make sure we are learning and sharing best practices and not allowing AI to do the learning for us.” In this course, any work you submit for credit must represent your own ideas and understanding of the assigned material. If you are uncertain about any case where your use of AI may be in conflict with University or course standards, please see me to discuss your concerns.

Any instance of dishonesty (including those detailed on the website provided above or in this syllabus) will ***immediately result in a grade of F for the entire course*** and will also be reported to The Chair of The Department of Chemistry & Biochemistry who will decide what the next steps may be.

Loyola University Absence Policy for Students in Co-Curricular Activities (including ROTC):

Students missing classes while representing Loyola University Chicago in an official capacity (e.g., intercollegiate athletics, debate team, model government organization) shall be allowed by the faculty member of record to make up any assignments and to receive notes or other written information distributed in the missed classes.

Students should discuss with faculty the potential consequences of missing lectures and the ways in which they can be remedied. Students must provide their instructors with proper documentation i.e., “[Athletic Competition & Travel Letter](#)” describing the reason for and date of the absence.

This documentation must be signed by an appropriate faculty or staff member and it must be provided to the professor in the first week of a semester. It is the responsibility of the student to make up any assignments. If the student misses an examination, the instructor is required to allow the student to take the examination at another time.

<https://www.luc.edu/athletheadvising/attendance.shtml>

Students who will miss class for an academic competition or conference must provide proper documentation to their instructor as early in the semester as possible.

Accommodations for Religious Reasons

If you have observances of religious holidays that will cause you to miss class or otherwise effect your performance in the class you must alert the instructor **within 10 calendar days of the first class meeting of the semester** to request special accommodations, which will be handled on a case by case basis.

Universal Absence Accommodation Policy

The purpose of a universal absence accommodation policy is to account for emergency circumstances (e.g., serious illness, caring for a family member, car accident) that require you to be absent from class, while maintaining fairness in grading for students who attend and complete all in-class graded assignments. We believe that class attendance and participation are essential for your success in this class, and that your health is important to us and our shared community. Please use good judgement and stay home if necessary/prudent for your circumstances.

Bring the issue to the attention of the instructors as soon as feasible and together we will decide how to best handle the situation.

Privacy Statement

Assuring privacy among faculty and students engaged in online and face-to-face instructional activities helps promote open and robust conversations and mitigates concerns that comments made within the context of the class will be shared beyond the classroom. As such, recordings of instructional activities occurring in online or face-to-face classes may be used solely for internal class purposes by the faculty member and students registered for the course, and only during the period in which the course is offered. Students will be informed of such recordings by a statement in the syllabus for the course in which they will be recorded. Instructors who wish to make subsequent use of recordings that include student activity may do so **only** with informed written consent of the students involved or if all student activity is removed from the recording. Recordings including student activity that have been initiated by the instructor may be retained by the instructor only for individual use.

Your well-being

If there are events occurring in your life that cause school to diminish in its priority, please discuss this with me or contact the Wellness Center (<http://www.luc.edu/wellness/index.shtml>) or the dean of students (http://www.luc.edu/studentlife/dean_of_students_office.shtml) for assistance. These are services that **your** tuition pays for and can be invaluable for your personal health and maintaining progress towards your degree. I am always willing to discuss how I can adapt the class and its materials so that you are successful.