CHEM 410A: Physical Chemistry, Spring 2025

Lecture Meetings: MWF 12:00-12:50 PM, GMCS-314
Instructor: Yuezhi Mao (he/him/his)
Email: ymao2@sdsu.edu
Office: GMCS 213D
Office hours: Tuesday/Thursday 4-5pm (tentative). The office hours will be in a hybrid format. Zoom link: https://SDSU.zoom.us/j/83188085837

Lab sections: Mon 2:00-4:40 PM (Yuezhi Mao); Wed 2:00-4:40 PM (Dr. David Pullman)
Lab Room: GMCS-245 (the chemistry computer lab) unless otherwise noticed
Note: A separate syllabus for CHEM 410A labs will be posted at a later time on Canvas, including a schedule for the labs.

Prerequisites: CHEM 232/232L, 251; MATH 252; PHYS 195/195L, 196/196L
Recommended: PHYS 197 and 197L

Textbook: *Physical Chemistry, 12th Edition* (Vol. 2) by Peter Atkins, Julio De Paula, and James Keeler (ISBN: 9780198851318). The electronic version of the textbook is available on Canvas ("*Day1Ready*" under "Modules"). In 410A we will cover Focuses 7-11, all in the 2nd volume of this book.

Lab manual: *Physical Chemistry Laboratory Projects Manual, Spring 2025*

CHEM 210:
CHEM 210 is a 1-unit course reviewing the required math background and the essential materials covered in 410A lectures. It can be viewed as a guided study session with the instructor (Mao) providing hints/helps. The course has no exams or homework: its grading is fully based on attendance and participation. Concurrent enrollment in CHEM 210 is *required* for students who have received below a "C" grade in any of the math and physics prerequisites. It is also **strongly recommended for all students** in this course, because 410A is a fast-paced class with very little time dedicated to problem-solving skills during the lectures.
The meeting time/location for CHEM 210 is Monday 1-1:50PM at GMCS 328. You are welcome to check it out in the first session (Jan 27) to see if you need to take it.

Course Overview:
CHEM 410A is the first half of the full-year Physical Chemistry course, focusing on **quantum mechanics and spectroscopy**. Following the 2nd volume of the Atkins book, we will first introduce the basic principles of quantum mechanics and apply them to describe translational, rotational, and vibrational motions of microscopic particles. We will then use our knowledge in quantum mechanics to (i) explore the structures of atoms and molecules, and (ii) interpret various types

of spectroscopies (rotational, vibrational, and electronic), which are essential experimental techniques for characterizing the composition and properties of chemical samples.

The lab component of this course involves predominantly **computer labs**, which are designed to reinforce some of the concepts covered in CHEM 410A lectures and to introduce several additional topics, including numerical integration, error propagation, linear and nonlinear fitting, and the use of Microsoft Excel (for data analysis) and Gaussian/GaussView (for simple quantum chemistry calculations).

Student Learning Objectives:

At the conclusion of this course, the students will be able to:

- Demonstrate a comprehensive understanding of the basic principles of quantum mechanics and apply the knowledge to model systems for describing translation, vibration, and rotation
- Utilize the fundamentals of quantum mechanics to calculate the electronic energy levels of atoms/simple molecules and relate the results to atomic/molecular spectra
- Build the connection between rotational/vibrational spectra and the quantum mechanical descriptions of the rotational and vibrational motions of diatomic and polyatomic molecules
- Interpret features in rotational, vibrational, and electronic spectra of simple molecules and extract molecular properties from spectroscopic data
- Identify the symmetry elements in common symmetric molecules and assign them to correct point groups
- Perform data analysis and curve fitting using Excel; conduct simple quantum chemistry calculations using Gaussian/GaussView; understand the uncertainties in data and the way errors propagate (through 410A labs)
- Be aware of the recent arguments around DEI initiatives among world-leading physical/theoretical chemists (published in *J. Phys. Chem. Lett.*) and express their own opinions on this

Course Modules (topics):

1. Focus 7A-7C: Basic principles of quantum mechanics
2. Focus 7D-7F: Model systems for translation, vibration, and rotation
3. Focus 8: Hydrogenic and many-electron atoms; atomic spectra
4. Focus 9: Molecular structure: VB and MO theory
5. Focus 11A-11B: General features of molecular spectroscopy; rotational spectra
6. Focus 11C-11D: Vibrational spectra
7. Focus 11F-11G: Electronic spectra
8. Focus 10A: Molecular symmetry

Course activities and grading scheme:

- **Lectures:** The lectures will take place during the regularly scheduled class time.

- **Lab projects (25%):** The labs start on the 2nd week of classes (the week of Jan 27). The detailed schedule of the labs will be posted on the Canvas page for CHEM 410A Labs (CHEM410A-02/03). The completion of the 12 lab projects and the lab practical accounts for 25% of your score for this course.
- **Midterm Exams (36%, 12% each):** There will be 3 exams during the semester, each having 100 points in total. You will have the full class period (50 mins) to finish. The tentative schedule is as follows:
    - Midterm 1: February 19 (Wed)
    - Midterm 2: March 21 (Fri)
    - Midterm 3: April 21 (Mon)
- **Final exam (20%):** The final exam for this course has been scheduled on **May 14, 10:30am-12:30pm**. It will have 200 points in total: the first 60 points will focus on the new materials after the 3rd midterm, and the remaining 140 points will be cumulative (covering the entire course).
- **Quizzes (12%):** Starting from the **2nd week** (Jan. 27), we will have quizzes roughly every two weeks at the end of the Monday lecture (see course calendar below). Each quiz will contain 10 points in total, and you will be given roughly 10 minutes to answer the questions. For each quiz, you will have **a second chance to work on it and resubmit it on Friday of the same week**. An answer key will be posted afterwards. Your resubmission will be graded on a 10-point scale, and the resulting score will then be scaled by 80% (i.e., the highest score you may get from retaking the quiz is 8/10). The accumulated points of six quizzes will amount to 12% of your final score.
- **Homework problems (5%):** Problem sets will be given roughly on a weekly basis. For each problem set, you are required to complete **all the *required* problems** (usually 4 in one single problem set) **plus one *elective* problem** unless otherwise noted. For each submission, **8 points will be given solely based on completion** (i.e., you will get the points as long as you worked on all the problems), and the other **2 points** will be based on the **correctness of one required problem** (which will be randomly selected each time). Solution keys will be provided after each problem set is due.
  IMPORTANT NOTE: While the homework problems only account for a small portion of your grade for this course, **completing the problems and going through the answer keys (once they are posted) are of the utmost importance for your success in this course**. Quantum mechanics turns out to be a challenging subject, both conceptually and technically. Therefore, you need to practice what you learned in the class via solving the problems.
- **Short essay related to the topic of diversity, equity, and inclusion (2%):** You will be asked to read two viewpoint articles recently published in *J. Phys. Chem. Lett.* and write a small essay (about one page long) to articulate your own opinions.

Tentative course calendar (for the lecture part only):

Week of	Mon	Wed	Fri
01/20	MLK Day (holiday)	Course Intro; Focus 7A	7A

01/27	7B; Quiz 1	7B	7B, 7C
02/03	7C	7C	7C, 7D
02/10	7D; Quiz 2	7D	7D, 7E
02/17	7E	Midterm 1	7E
02/24	7E, 7F.1; Quiz 3	7F.1	7F.2
03/03	7F.2	8A	8A
03/10	8A; Quiz 4	8A, 8B	8B
03/17	8B, 8C	8C	Midterm 2
03/24	8C, Focus 9 prologue	9A, 9B	9B
03/31	Spring break (no class)		
04/07	9C; Quiz 5	9D	9D, 9E
04/14	9E, 11A	11A	11B
04/21	Midterm 3	11B, 11C	11C
04/28	11D; Quiz 6	11F	11F, 11G
05/05	11G, 10A	10A	No class
05/12	No class	Final Exam	

Note: This schedule is only *tentative* (primarily to show you what will be covered in this course). Any important changes to the schedule (e.g., shift of midterm dates, Zoom/pre-recorded lectures instead of in-person class, etc.) will be announced well in advance on Canvas.

Tentative grading scale:

Letter	% Cutoff	Letter	%Cutoff
A	88	C	58
A-	83	C-	53
B+	78	D+	48
B	73	D	44
B-	68	D-	40
C+	63	F	<40

Note: The grading scale above is only a rough example. The final cutoffs may be adjusted based the overall grade distribution of the class.

Late Policy:

The following late policy applies to the assignments in the lecture part of this course only: if your submission is late by

- 0-2 hours: grace period; no deduction
- 2-24 hours: 25% deduction
- Every 24 hours past due: deducting 25% of the total *in addition to* the initial 25%

For example, under this rule there will be a 25% deduction if your submission is late by 10 hours, 50% deduction if late by 30 hours, and so forth. No points will be given if your submission is late by more than 4 days.

Note: The deduction due to late submission may be waived upon the instructor's approval if (i) the instructor is informed in a written form (e.g., email) *before* the assignment is due, and (ii) there is a legit, excusable reason (based on the instructor's judgment) for not being able to turn in the work on time.

Add/Drop Procedure: The add/drop deadline is **February 3, 2025**. Please refer to https://registrar.sdsu.edu/students/registration for full details.

Academic honor code:

Students are expected never to represent someone else's work as their own or assist others in doing so. Violations of this rule will be documented and may result in automatic failure and disciplinary review by the University. Please see the SDSU academic honesty page for further information.

Essential student information:

For essential information about student academic success, please see the SDSU Student Academic Success Handbook.

- SDSU provides disability-related accommodations via the Student Ability Success Center (sascinfo@sdsu.edu | sdsu.edu/sasc). Please allow 10–14 business days for this process. Please note that accommodations are not retroactive, and that the instructor cannot provide accommodations based on disability until an accommodation letter is received.
- Class rosters are provided to the instructor with each student's legal name. Please let the instructor know if you would prefer an alternate name and/or gender pronoun.

Land acknowledgment:

For millennia, the Kumeyaay people have been a part of this land. This land has nourished, healed, protected and embraced them for many generations in a relationship of balance and harmony. As members of the San Diego State University community, we acknowledge this legacy. We promote this balance and harmony. We find inspiration from this land, the land of the Kumeyaay.

Diversity, equity, and inclusion:

We, at SDSU, value the diverse identities of our students, faculty, and staff, which include but are not limited to the differences in race, gender, ethnicity, sexual orientation, age, socioeconomic status, religion, and disability. We will work together to promote diversity, equity, and inclusion in our learning environment, not only for academic excellence but also for social justice. The instructor is committed to adopt an inclusive teaching approach to help students from diverse backgrounds succeed in this course. Discussions where distinct perspectives and opinions are respected and valued are encouraged inside and outside the classroom.

Physical Chemistry Lab, Chem 410A

GMCS-245

Session 1 – Mon., 2:00-4:40 pm

Session 2 – Wed., 2:00-4:40 pm

Attendance required

Instructors:

Yuezhi Mao (Mon. Session): ymao2@sdsu.edu

David Pullman (Wed. Session): dpullman@sdsu.edu

Teaching assistant: Jo Charlonis

Lab manual: **Physical Chemistry Laboratory Projects Manual (Spring 2025). IMPORTANT: The printed version of lab manual is required. Please get that from the bookstore before the first lab.**

The main syllabus for Chem 410A will be provided by Dr. Pullman in the lecture part of the course. This lab part will be **25%** of your final grade for Chem 410A.

The lab part of Chem 410A consists of 12 projects. The programs you will use are Excel (either 2013 or 2016, but almost any version could be used) and Gaussian 16. These are very practical programs that every student should learn. Excel will allow you to do calculations very easily and graph results that are presentable enough for publication. Gaussian is a powerful and widely used program for calculating minimum energy structures of molecules. You will find that what you learn in this lab will help you in other classes, in research, and in future jobs. ***Please do not use Google Sheets for the Excel projects***.

The project instructions that you will find in this manual step you through specific procedures. These can be started before class but must be finished by the end of the class period, along with any assignment given during class (either 5:00 pm on Monday or 5:00 pm Wednesday, depending on your section). The projects are designed to take 2 to 2 ½ hours. Those students who have experience with Excel may be able to finish more quickly, but if you are worried that you will have trouble finishing before the deadline (5:00 pm), you may want to start working before class, or at least look through the manual.

For almost every project an additional assignment handout will be given during the class period. This part must be done independently; it will test your understanding of the procedures and concepts.

You will get much more out of the class if you can work things out on your own. In particular, if you don't get a result that you expect, take some time to "troubleshoot" before asking for help from other students or the instructor. The more you try, the better you will get at

it. Although the instructors will be happy to help, as the semester progresses, they expect students to have learned some troubleshooting techniques and may start to require more independent problem-solving.

Daily schedule in the computer lab

There will be a short (~15 minutes) lecture/demonstration for each project. Be sure to pay attention to this introduction even if you have already started the project. Some of the information will be important for you to finish the project correctly and efficiently. After the introduction, we will move around the room answering questions and helping with trouble-shooting. When you are ready, you can start any extra handout required for the project. This part must be worked out independently of other students. At this point, we will not help you with troubleshooting questions (for example, "Why doesn't this work?"), but you can still ask questions. This is your chance to work things out on your own!

Near the end of class, the instructor will again help out with troubleshooting for those students who need it. Some of you may be done by this time. If you are not finished by 4:40 PM, you may continue working until 5:00 PM, but the instructor might not be available to help after 4:40 pm.

A fundamental rule when working with computers is that **you should save your work on a regular basis**. How often you do this depends on how frequently you have made changes to your document or worksheet. It can be *intensely* frustrating if the computer crashes and you have not saved your work.

Tentative Schedule

Week	Mon	Wed
1 (Jan. 20)	No lab	No lab
2 (Jan. 27)	Lab 1	Lab 1
3 (Feb. 3)	Lab 2	Lab 2
4 (Feb. 10)	Lab 3	Lab 3
5 (Feb. 17)	Lab 4	Lab 4
6 (Feb. 24)	Lab 5	Lab 5
7 (Mar. 3)	Lab 6	Lab 6

8 (Mar. 10)	Lab 7	Lab 7
9 (Mar. 17)	Lab 8	Lab 8
10 (Mar. 24)	Lab 9	Lab 9
11 (Mar. 31)	Spring break (no lab)	
12 (Apr. 7)	Lab 10	Lab 10
13 (Apr. 14)	Lab practical	Lab practical
14 (Apr. 21)	Lab 11	Lab 11
15 (Apr. 28)	Lab 12	Lab 12
16 (May. 5)	No lab	No lab

The list of lab projects:

Lab 1. Introduction to Microsoft Excel

Lab 2. Introduction to Microsoft Excel (cont)

Handout for Parts 2 and 3 will be given in class.

Lab 3. Numerical Integration and the Particle in a Box

Handout with data and a function for Part 3 will be given in class

Lab 4. UV-Visible and Noise spectra/Intro to Error analysis

Handout with data for Part II will be given in class

Lab 5. Instrumental Noise/Propagation of error

Handout for Part D will be given in class

Lab 6. Propagation of Errors (cont)

Handout for Part 3 will be given in class

Lab 7. Fitting a Straight Line to Data

Handout for Part 2B will be given in class

Lab 8. Fitting a Straight Line to Data (cont)

Handout for Parts 2 and 3 will be given in class

Lab 9. Nonlinear Least–squares Fitting of Data

Handout for Part 3 will be given in class

Lab 10. Nonlinear Least–squares Fitting (cont.)

Handout for Part 2 will be given in class

Lab 11. Molecular Modeling with Gaussian/Gauss View

An answer sheet will be handed out in class

Lab 12. Generating a Potential Energy Curve

A handout will be given in class

The detailed content of each lab project can be found on the Lab Manual.

Each project should be done in a single Excel Workbook (using as many "sheets" as necessary). Submit the finished file by 5:00 pm on the day of your lab section. The submission will close at 6 pm. One point will be deducted for late submissions between 5 and 6 pm. The format of your filenames should be similar to: lastname_#.xlsx. Your submission for each lab project will be graded on a 15-point scale, except for Lab 1 (which is worth 10 points).

Please do not send your files to any other students. If we find that you are using another student's Excel file for your purposes, both you and the other student will receive a zero for that project. Everyone should be constructing their own worksheets without using any sort of template.

Lab Practical

A lab practical is planned after Lab 10 (the last Excel project), in which **you will complete a series of tasks using Excel independently, without any help from the instructor or peers**. It will be administered in an exam setting. Its goal is to assess your proficiency of the Excel skills covered in the previous weeks. The points associated with the lab practical will be equal to two regular labs (i.e., 30 points).

Lab #4 in CSL-222

Lab #4 includes a "wet" lab component that takes about 30 minutes. Safety apparel will be required.

Lab Makeups

Lab attendance is required while doing the second parts of the projects (handouts). If you miss a lab because of a personal crisis, notify the instructor immediately by email, and we will try to schedule a makeup time for finishing the assignment handout.

Note: Make-ups must be arranged within one week of the assignment.