CHEM 410A: Physical Chemistry, Fall 2023

Instructor: Yuezhi Mao (he/him/his)
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Office: GMCS 213D (Phone #: 619-594-1617)
Lecture Meetings: MWF 9:00–9:50 AM, GMCS-309

Lab instructors:

- Dr. Karen Peterson (office: CSL-309; email: kpeterson@sdsu.edu)
- Dr. David Pullman (office: CSL-301; email: dpullman@sdsu.edu)

Lab time: Section 1: Mon 2:00–4:40 PM; Section 2: Wed 2:00–4:40 PM
Lab Room: GMCS-245 (the computer lab)

Office hours (Mao): Tuesday 3-4pm & Thursday 11am-noon, or by appointment. The office hours will be in a hybrid form. Zoom link: https://SDSU.zoom.us/j/83635413808

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: 9781726908658). In 410A we will cover Focuses 7–12, all in the 2nd volume.

Lab notes: *Physical Chemistry Laboratory Projects Manual, Fall 2023*
(ISBN: 9781726908658)

CHEM 210:
CHEM 210 is a 1-unit course (instructor: Dr. Karen Peterson) reviewing the essential math background knowledge and skills needed in CHEM 410A. It is a workshop class, *with only an attendance/participation requirement with no exams or homework*. Concurrent enrollment 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 unless you are confident with your math capabilities. The meeting time for 210 is Monday 1PM, and you are welcome to check it out on the first day of class and see if you need to take it. (Note: the 410A lectures have a lot to cover and thus will have no time dedicated to math reviews.)

Course Overview:
CHEM 410A is the first half of the full-year Physical Chemistry course focusing on **quantum mechanics (QM) and spectroscopy**. Following the 2nd volume of the Atkins book, we will first introduce the basic principles of QM and use them to describe the translational, rotational, and vibrational motions of microscopic particles. We will then extend our knowledge of QM by

investigating the electronic structure and nuclear motions of atoms/molecules. After a relatively brief discussion of molecular symmetry and group theory, we will apply what we learned about QM to elucidate the fundamentals of various types of spectroscopies, including rotational, vibrational, electronic, and nuclear magnetic resonance (NMR) spectroscopies, which are key techniques that are utilized to characterize the components 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 lectures and also to introduce several additional topics, including error analysis, curve fitting, and the use of Microsoft Excel (for data analysis) and the Gaussian/GaussView (for simple quantum chemistry calculations).

Student Learning Objectives:

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

- Articulate the basic principles of quantum mechanics and apply them to simple model systems such as particle in a box, harmonic oscillator, rigid rotor, etc.
- Use the fundamentals of quantum mechanics to calculate the electronic energy levels of atoms/simple molecules and relate the results to atomic/molecular electronic spectra
- Build the connection between observed rotational/vibrational spectra and the quantum mechanical descriptions of the rotational and vibrational motions of diatomic and polyatomic molecules
- Identify the point group of common symmetric molecules and the involved symmetry elements and operations; understand the basic concepts in group theory and the meaning of symmetry labels for molecular orbitals/vibrations
- Develop a working knowledge of the quantum theories underpinning electronic, rotational, vibrational, and NMR spectroscopy
- Perform data analysis and curve fitting using Excel and simple quantum chemistry calculations using Gaussian/GaussView; understand the uncertainties in data and the way errors propagate (through labs)
- Be aware of the recent arguments around DEI initiatives among world-leading physical/theoretical chemists published in *J. Phys. Chem. Lett.* and develop 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, rotation, and vibration
3. Focus 8: Hydrogenic and many-electron atoms; atomic spectra
4. Focus 9: Molecular structure, with a focus on the molecular orbital theory
5. Focus 10A-10B: A “gentle” introduction to molecular symmetry and group theory (will be less involved compared to the textbook)
6. Focus 11A-11B: General features of molecular spectroscopy; rotational spectra
7. Focus 11C-11D: Vibrational spectra
8. Focus 11F-11G: Electronic spectra
9. Focus 12: NMR spectra and electron paramagnetic resonance

Course activities and grading scheme:

- **Lectures:** The lectures will take place during the regularly scheduled class time.
- **Lab projects (25%):** The labs start during the first week of classes. *Do not miss the first day*: there will be an introductory project that will be graded (if you do not attend, you must contact Dr. Pullman or Dr. Peterson within one week after the first lab). For detailed schedule please see the Canvas page for 410A lab. The completion of the lab projects accounts for 25% of your score for this course.
- **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:
    - Exam 1: Wednesday, Sept. 20
    - Exam 2: Wednesday, Oct. 18
    - Exam 3: Monday, Nov. 13
- **Final exam (20%):** The final exam for this course has been scheduled on Dec. 13, 8–10am. It will have 200 points in total: the first 60 points will focus on the materials not covered by previous exams and the rest will cover the entire course.
- **Quizzes (10%):** Starting from the 2nd week (Aug. 28), we will have quizzes every Monday, except during the weeks when there is an exam (in cases when Monday is a holiday, the quiz will take place on Wed instead). Each quiz will contain 10 points in total and you will be given 5 minutes to complete the questions. The accumulated points will amount to 10% of your final score.
- **Homework problems (6%):** A problem set will be given for each course module listed above. You are required to (i) submit your work for 3 problems (on paper, 3 points each) and (ii) identify one problem that you find most difficult and describe the troubles you encounter/overcome (1 point). You will get 10 points from each submission based solely on completion. Solution keys will be provided after the problem set is due. **IMPORTANT NOTE:** While the homework problems only account for a small portion of your grade, **completing the problems is of the utmost importance for your success in this course**. Quantum mechanics is a challenging subject, both conceptually and technically, and thus you will need to practice what you learned in the class via solving the problems.
- **Miscellaneous:**
    - **Small essay related to the topic of diversity, equity, and inclusion (3%):** You will be asked to read two viewpoint articles recently published in *J. Phys. Chem. Lett.* and write a small essay (half to one page) to articulate your opinions
    - **Office visits (1% bonus):** All students are encouraged to attend the office hour sessions (twice a week). In some of these I will provide mini reviews going over the class materials. If you come to office hours >= 4 times during the semester, you will get 1% bonus which will be added to your final percentage score.

Tentative course calendar (for the lecture part only):

Week of	Mon	Wed	Fri
08/21	Course intro; Focus 7A	7A	7B
08/28	7B, 7C	7C	7C
09/04	Labor Day (no class)	7D	7D
09/11	7E	7E	7E, 7F
09/18	7F	Exam 1	7F, 8A
09/25	8A	8A, 8B	8B
10/02	8B	8C	8C
10/09	8C, 9A	9B	9C
10/16	9D	Exam 2	9E
10/23	9E, 9F	10A	10A, 10B
10/30	10B	10B, 11A	11A
11/06	11B	11B	Veterans Day (no class)
11/13	Exam 3	11C*	11C, 11D*
11/20	11D	Thanksgiving break	Thanksgiving break
11/27	11F	11F, 11G	12A
12/04	12A, 12B	12B	12D, Review
12/11	Review	Final Exam: 8-10am	

* The instructor will be traveling for a conference between Nov. 15-18 so there will be no in-person lectures on Nov. 15 (W) and 17 (F). Pre-recorded videos will be posted for these two lectures.

Note: This schedule is only *tentative* (primarily to show you what will be covered in this course). Important adjustments to the schedule will be posted on Canvas under "Announcements".

Tentative grading scale:

Letter	% Cutoff	Letter	%Cutoff
A	89	C	60
A-	84	C-	55
B+	80	D+	50
B	74	D	45
B-	70	D-	40
C+	65	F	<40

Note: The grading scale above is only a rough example. Your final grade may be influenced by the overall class grade distribution to reflect your rank in comparison with your peers.

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: 20% deduction
- Every 24 hours past due: deducting 20% of the total *in addition to* the initial 20%

For example, under this rule there will be a 40% deduction if your submission is late by 30 hours, and a 60% deduction if late by 50 hours, and so forth.

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 *September 1, 2023*. 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 the 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.