CHEM 410A: Physical Chemistry, Spring 2024

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 3-4:30pm (or by appointment). The office hours will be in a hybrid form. Zoom link: https://SDSU.zoom.us/j/82630982243

Lab instructor: Matthew Campbell (email: mmcampbell@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) unless otherwise noticed

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). In 410A we will cover Focuses 7-11, all in the 2nd volume.

Lab notes: *Physical Chemistry Laboratory Projects Manual, Spring 2024* (ISBN: 9781726909037)

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 (me) providing hints/helps), and *the grading is fully based* on *attendance and participation 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, 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 Friday 1-1:50PM at GMCS 306. You are welcome to check it out in the first session (Jan 19) and 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 the description of translational, rotational, and vibrational motions of microscopic particles. We will then utilize our knowledge in quantum mechanics to (i) explore the structures of atoms and molecules and (ii) interpret various types of spectroscopies (including rotational, vibrational, and electronic spectroscopies),

which are crucial 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 lectures and also to introduce several additional topics, including error analysis, curve 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 important model systems for 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 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, rotation, and vibration
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 during the first week of classes. *Do not miss the first lab*: there will be an introductory project that will be graded (if you do not attend, you

must contact Matt Campbell 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.

- **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: Wednesday, Feb. 14
    - Midterm 2: Monday, Mar. 18
    - Midterm 3: Monday, April 15
- **Final exam (20%):** The final exam for this course has been scheduled on May. 8, 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 rest 140 points will be cumulative (covering the entire course).
- **Quizzes (10%):** Starting from the **2nd week** (Jan. 22), we will have quizzes at the end of every Monday lecture, except for the weeks during which exams are scheduled. Each quiz will contain 10 points in total, and you will be given roughly 8 minutes to answer the questions. For each quiz, you will be given a **second chance to work on it and resubmit it during the Friday class**, after which an answer key will be provided. I will re-grade your resubmission on a 10-point scale and multiply the number by 80%. The accumulated points will amount to 10% of your final score.
- **Homework problems (7%):** 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, you will get **6 points based solely on completion** (i.e., no problems skipped), and the other **4 points** will be based on my **grading of one required problem** (which will be randomly selected). 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. Hence, 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 (half to one page long) to articulate your own opinions.

Tentative course calendar (for the lecture part only):

Week of	Mon	Wed	Fri
01/15	MLK Day (holiday)	Course Intro; Focus 7A	7A
01/22	7B	7B	7B, 7C
01/29	7C	7C	7C

02/05	7D	7D	7D, 7E
02/12	7E	Midterm 1	7E
02/19	7E, 7F.1	7F.1	7F.2
02/26	7F.2	8A	8A
03/04	8A	8B	8B
03/11	8B, 8C	8C	8C, Focus 9 Prologue
03/18	Midterm 2	9A, 9B	9B
03/25	9C	9D*	9D, 9E
04/01	Spring break (no class)		
04/08	9E, 11A	11A	11B
04/15	Midterm 3	11B, 11C	11C
04/22	11D	11F	11F, 11G
04/29	11G, 10A	10A	No class
05/06	No class	Final Exam	

* The instructor will be visiting CSU Long Beach to give a seminar on March 27 so there will be no in-person class on that day. Pre-recorded lecture will be posted instead.

Note: This schedule is only *tentative* (primarily to show you what will be covered in this course). Important changes to the schedule (e.g., shift of midterm dates, additional Zoom/pre-recorded lectures in place of in-person class) will be posted well in advance through Canvas announcements.

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. 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: 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 *January 26, 2024*. 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.