Chemistry 410A: Physical Chemistry

Course Syllabus

Fall 2024, Mon, Wed, and Fri 12:00 to 12:50, GMCS-314

Instructor Dr. David Pullman, CSL–301, 619–594–5573, dpullman@sdsu.edu

Office Hours Mon 8:00–9:00 PM by zoom (link will be provided); Wed 1:00–2:00 PM in CSL-301

Textbook Physical Chemistry, 12th Ed., Vol. 2, P.W. Atkins, J. de Paula, and J. Keeler, Oxford

University Press. Both print book and ebook versions are available. Purchasing either one gives you access to additional resources located on the Oxford Learning Link

website.

Prerequisites Chemistry 232, 232L, 251; Mathematics 252 (Mathematics 150, 151; 252 or Physics 195,

195L, 196, 196L for chemistry teaching major); Physics 195, 195L and 196, 196L. Recommended: Physics 197 and 197L and Chem 210 (210 is required if you received a

C– or lower in any of the the math or physics prerequisite classes)

Catalog Description

Theoretical principles of chemistry with emphasis on mathematical relations. Theory and practice in acquisition and statistical analysis of physical measurements on chemical

systems.

Course Overview The focus of the lecture portion of Chem 410A is on Quantum Mechanics and its main application, spectroscopy. After developing the basic principles of Quantum Mechanics to describe the translational, vibrational, and rotational motion of particles, we will extend our knowledge to understand the motion of electrons and nuclei in atoms and molecules. This knowledge of atomic and molecular properties will lead in a natural way to a discussion of various types of spectroscopy (including rotational, vibrational, electronic, and nuclear magnetic resonance spectroscopy), which are key techniques in modern science for analyzing chemical samples.

The computer lab portion of Chem 410A is designed to reinforce some of the concepts from the lecture and to introduce additional topics, such as error analysis and curve fitting, which are important in the analysis of scientific data. You will use Microsoft Excel and Gaussian to carry out the scientific calculations. Further details are given in the lab handouts.

Topics The two topics we will cover in Chem 410A are Quantum Mechanics and Spectroscopy.

Quantum Mechanics Chapter 7 ("Focus 7") Quantum Theory

Chapter 8 ("Focus 8") Atomic Structure and Spectra

Chapter 9 ("Focus 9") Molecular Structure

Spectroscopy Chapter 11 ("Focus 11") Molecular Spectroscopy

Chapter 12 ("Focus 12") Magnetic Resonance

Course Structure Chem 410A consists of three hour-long lectures each week in addition to a three hour computer lab each week. The lectures will roughly follow the text, with additional material occasionally added. Lecture notes will be posted on Canvas ahead of time.

Exams Exam 1 Chapter 7; tentatively Mon, Sept 23

Exam 2 Chapter 8; tentatively Fri, Oct 18

Exam 3 Chapter 9; tentatively Wed, Nov 13

Final Chapter 11, 12 and cumulative Wed, Dec 18, 10:30–12:30

Occasional quizzes will also be given

- Exams (except the final exam) and quizzes will be given during the lecture hour
- No makeup exams (or quizzes) will be given.
- Dedicated calculators may be used during exams and quizzes; cell phones and other electronic gadgets, like ipods or ipads, **cannot** be used during the exams or quizzes.

Problem Sets

There will be one or two problem sets per chapter. Problem sets will <u>not</u> be graded; you do not need to hand them in. You can download them from the Canvas website for Chem 410A. Solution keys will generally be posted about one week after the problem sets have been posted. <u>Doing the problem sets is of the utmost importance to learning the</u> material and doing well on quizzes and exams.

The **BAD**, but easy, way to do a problem is to look at the solution while you think about the problem. Nearly as bad is to think about a problem for five minutes, give up, and then look at the solution key. You are doing yourself a substantial disservice if you approach the problem sets in this fashion.

The **GOOD**, but more difficult, way is to focus your energy on a problem for a sustained period (say 30 minutes). If you can't answer the problem, go on to another problem—but do not look at the answer key if it is already available. Later on, after you have done other problems, things may gel in your mind, and you may see how you should approach the problem. **Real learning involves, among other things, recognizing patterns in problems and comes only after a significant effort on the part of your brain.**

Canvas

Canvas will be used to post announcements and course documents (problem sets, solution keys to problem sets, exams, and quizzes, etc.).

Grading

Exams(3)	15% each	24404
Final	20% total	Lecture part of $410A = 75\%$
Quizzes	10% total	
Computer Lab	25%	

Final grades, +/- grading and curved scale will be used.

Student Learning Outcomes

Upon completing Chem 410A, students will be able to:

- 1. Articulate the basic principles of Quantum Mechanics, as well as the differences between Classical and Quantum Mechanics
- 2. Use the fundamental model systems of Quantum Mechanics to calculate or estimate properties of real atoms and molecules
- 3. Interpret atomic and molecular spectra in terms of the energies and motions of atoms and molecules
- 4. Perform scientific calculations and simulations using Excel and Gaussian
- 5. Describe contributions and perspectives of Physical Chemists from varying backgrounds

Add/Drop Procedure

The add/drop deadline is Monday Sept. 9, 2024 at 11:59 PM. For details, see https://registrar.sdsu.edu/students/registration

Students with Disabilities

If you are a student with a disability and believe you will need accommodations for this class, it is your responsibility to contact Student Disability Services at (619) 594-6473. To avoid any delay in the receipt of your accommodations, you should contact Student Disability Services as soon as possible. Please note that accommodations are not retroactive, and that accommodations based upon disability cannot be provided until you have presented your instructor with an accommodation letter from Student Disability Services. Your cooperation is appreciated.

Academic Honesty

Cheating amounts to lying because you are saying that you did the work as instructed whereas, in fact, you did not. Cheating will not be tolerated and will result in grade reduction. It will also be documented according to university rules (see https://sacd.sdsu.edu/student-rights/academic-dishonesty).