Chemistry 410A: Physical Chemistry

Course Syllabus

Fall 2018, Mon, Wed, and Fri 12:00 to 12:50, GMCS–308

Instructor       Dr. David Pullman, CSL–301, 619–594–5573, dpullman@sdsu.edu
Office Hours     Mon, Tues, and Wed from 1:00–2:00 in CSL–301
Textbook         Physical Chemistry, 10th Ed., P.W. Atkins and J. de Paula
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

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, Maple, and Gaussian to carry out the scientific calculations. Further details are given in the lab manual, available in the bookstore.

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

Quantum Mechanics
- Chap 7 Introduction to Quantum Theory
- Chap 8 The Quantum Theory of Motion
- Chap 9 Atomic Structure and Spectra
- Chap 10 Molecular Structure

Spectroscopy
- Chap 12 Rotational and Vibrational Spectra
- Chap 13 Electronic Transitions
- Chap 14 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.

Exams
- Exam 1 Tentatively chapters 7 and 8
- Exam 2 Tentatively chapters 9 and 10 (might be split into quiz for 9 and exam for 10)
- Exam 3 Tentatively chapters 12 and 13
- Final Tentatively chapter 14 and cumulative Fri, Dec 14, 1:00–3:00, GMCS–308

• No makeup exams (or quiz) will be given.
• Dedicated calculators may be used during exams and quizzes; cell phones and other electronic gadgets, such as ipods and ipads, must be turned off before the start.
Problem Sets

You can download them from the Blackboard website for Chem 410A. In general, there will be one or two problem sets per chapter. Each problem set will have approximately ten problems. A few (1 to 3) of these will be chosen at random for grading. On the due dates, the problem sets should be handed in at the beginning of the class period. They will usually be worth 100 points. Late problem sets will be marked off 20 points. Generally, answer keys will be posted on Blackboard after the next class. Problem sets will not be accepted after the answers have been posted! Doing the problem sets is of the utmost importance to learning the material and doing well on exams. Real learning involves, among other things, recognizing patterns in problems and comes only after a significant effort by your brain.

Blackboard

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

Grading

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<tr>
<td>Exams(3)</td>
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<td>Final</td>
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<td>Lecture part of 410A = 75%</td>
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<td>Problem Sets</td>
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<td>Computer Lab</td>
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<td>Final grades, +/- grading and curved scale will be used.</td>
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Student Learning Outcomes

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, Maple, and Gaussian

Add/Drop Procedure

The add/drop deadline is Monday Sept. 10, 2015. For details, see http://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 the Student Ability Success Center (SASC) at (619) 594-6473. To avoid any delay in the receipt of your accommodations, you should contact SASC 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 SASC. Your cooperation is appreciated.