CHEM410A-01-02-CX-Fall2022

Chem 410A, Physical Chemistry, Fall 2022

Lecture: MWF 9:00 – 9:50 AM
Room: GMCS-309

Lab: Session 1 - Monday, 2:00-4:40
Session 2 - Wednesday, 2:00-4:40
Room: GMCS-245

Instructors:

Lecture
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Lab
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Office hours (Peterson) Monday, 10:00 – 11:00 am, CSL-309
Thursday, 8:00 – 9:00 pm, Zoom

Meeting ID: 853 0948 6202

https://SDSU.zoom.us/j/85309486202 (Links to an external site.)

Catalog Course Description: CHEM 410A. Physical Chemistry (4) Three lectures and three hours of laboratory. Prerequisites: Chemistry 232, 232L, 251; Mathematics 252; Physics 195, 195L, 196, 196L. Recommended: Physics 197 and 197L. Theoretical principles of chemistry with emphasis on mathematical relations. Theory and practice in acquisition and statistical analysis of physical measurements on chemical systems.

Textbook

The required textbook for this course is ***Physical Chemistry, 11th Edition*** by Peter Atkins, Julio de Paula, and James Keeler (ISBN: 978-0-19-876986-6). We will be covering Focus 7, 8, 9, 10, 11, 12

Lab Manual

The lab projects will be handed out and/or posted in Canvas out each week. Do not use lab handouts or manuals from previous semesters because changes may have been made.

Overview

This first semester of a full-year course in Physical Chemistry covers quantum chemistry and spectroscopy. The second semester covers thermodynamics, kinetics, reaction dynamics, and some statistical mechanics. Quantum chemistry is a challenging subject, both mathematically and conceptually, but it is a critical foundation for understanding the underlying features of both experimental spectroscopy and theoretical computations. Spectroscopy is used in all areas of chemistry as a method for analyzing samples to determine what is there and how much. It is also used to measure molecular properties directly. As for any difficult subject, learning quantum chemistry requires one to experience the ideas many times and in many different ways, through reading, doing problems, conducting experiments and discussions with others. My approach in this class is to encourage all of this through a variety of assignments. The handout you will receive for each chapter outlines the reading and gives problems directly based on the reading. It is important to read the material and at least try the relevant problems before coming to class, so that the lecture becomes a means of clarifying what you have seen, rather than a first-time introduction. I don't expect you to understand everything you have read, but I do expect you to make a serious attempt. I think you will find that you get much more out of the lecture when you have had a pre-exposure to the ideas!

Learning Outcomes

By the end of the course, you will have learned the following:

- Understand the relationship between first principles in quantum mechanics and the properties of molecules, in particular their geometric and electronic structure.
- Be able to calculate rotational energies of molecules and relate the energy level separations observed spectra and to the molecular structure
- Be able to calculate the vibrational energies of molecules and relate the energy level separations to observed spectra and to the force constants of the molecular bonds.
- Be able to calculate molecular electronic energies in simple cases and to learn the underlying principles of advanced computational methods
- Understand the fundamentals of spectroscopic methods and how they relate to theories of quantum mechanics.
- Develop a working knowledge of NMR theory.
- Be able to do calculations using Excel, Maple and Gaussian programs. (Lab part of class)
- Understand uncertainties in data and be able to propagate uncertainties to the final result (Lab part of class)

Chem 210: This is a one-unit course that is required for students who have received below a C grade in any of the math and physics prerequisites. It is also recommended for students who feel that they need extra help with the mathematics component of this course. The meeting time is Monday at, 1:00 pm. More information will be given on the first day of the Chem 410A class.

Lectures

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

Chapter handouts

For each module, you will be given a handout that will guide you in your reading, provide problems for practice and understanding, and serve as a study guide for exams. The problems labelled "Q" are intended to be straightforward, although not always easy, and should be at least attempted immediately after reading the relevant section of the book. This will help you to better understand what you just read. Even if you aren't able to figure out the answer, trying the problem will help you on the daily quiz. The problems at the end of the handout (labelled "P") are generally more comprehensive and will help test your understanding.

Canvas discussion:

Each problem in the handout will be assigned to a specific person to solve in detail and post in the Discussion section in Canvas. A good attempt at the answer must be posted before the next class period after the problem is assigned; there is a one-point penalty for posting an initial attempt after this time. After the initial post, other students can comment, make suggestions, ask questions, and even post their own answer. The deadline for posting a complete answer to your assigned problem is usually one week after the assignment date, but may be sooner near exam time. Even if another student answers the question correctly, you must post your own correct answer to receive credit. Only the final submission will be graded; if other students have already given answers, summarize their results into a neat, readable, and complete final version. For full credit (8 points), your answer should be well written with the steps in any calculations explained. As part of the assignment, I also expect you to answer any questions other students may have about your problem after it is posted. These posted answers constitute an answer key.

Extra credit: Extra points will be given for helpful contributions to the Discussion Board regarding problem solutions. If you see that an answer is incorrect or unclear, post your comment so that the author has a chance to correct it. Each person can get a maximum of 10 extra-credit points for the semester.

Daily Quizzes

A short (~5 minute) quiz will be given at the beginning of class every day. It will usually cover the reading and problems assigned at the end of the previous class. There will be a total of about 40 quizzes given for 3 points each. The best 33 of these will be used toward your grade.

Homework Assignments

Throughout the semester I may have homework assignments. These generally will involve problems that require Excel or substantial mathematical work.

Exams

There will be three exams during the semester. These will be administered in class, and you will have the full class period to finish. The tentative schedule is as follows:

Exam I Friday, Sept. 16

Exam II Wednesday, Oct. 12

Exam III Wednesday, Nov. 19

Final exam
The final exam takes place on Wednesday, Dec. 14, 2021, 8:00 – 10:00 AM. The exam will have one section covering the last 3-4 weeks of the class, and another section that will be cumulative.

Grading

Three exams 300 pts (100 pts each)
Final exam 150 pts
Daily quizzes 99 pts (3 pts each; best out of 33)
Discussion questions ~56 pts (8 pts each; ~ 7 assigned questions)
Homework assignments ~30 pts
Lab projects: 160 - 175 pts
Total: ~800 pts

The grading scheme will be as follows:

A	89-100%	C	59-66%
A-	85-89%	C-	55-59%
B+	81-85%	D+	50-55%
B	74-81%	D	44-50%
B-	70-74%	D-	40-44%
C+	66-70%	F	< 40%

Topics/Modules

Module 1. Prologue
Module 2. Focus 7A,B,C Quantum Theory; Introduction

Module 3. Focus 7D,E,F Quantum Theory; Examples
Module 4. Focus 8 Atomic Structure and Spectra
Module 5. Focus 9 Molecular Structure
Module 6. Focus 10 Molecular Symmetry (10A – 10B)
Module 7. Focus 11A,B Molecular Spectroscopy; General Features, Rotational Spectroscopy
Module 8. Focus 11C,D,E Molecular Spectroscopy; Vibrational Spectroscopy
Module 9. Focus 11F,G Molecular Spectroscopy; Electronic Spectroscopy
Module 10. Focus 12 Magnetic Resonance

Lab Module. Computer Lab Projects

Lab projects

The labs start during the first week of classes – do not miss the first day. The following list of projects is tentative.

Lab 0 Introduction to Microsoft Excel
Lab 1 Introduction to Microsoft Excel (cont.)
Lab 2 Numerical Integration and the Particle in a Box
Lab 3 UV-Visible Spectra/Introduction to Error Analysis
Lab 4 Instrumental Noise/Propagation of Error
Lab 5 Propagation of Error (cont.)
Lab 6 Fitting a Straight Line to Data
Lab 7 Nonlinear Least–squares Fitting of Data
Lab 8 Nonlinear Least–squares Fitting (cont.)
Lab 9 Fitting a Straight Line to Data (cont.).
Lab 10 Molecular Modeling with Gaussian/GaussView
Lab 11 Generating a Potential Energy Curve
TBA

Add/Drop Procedure: The add/drop deadline is Sept 2, 2022. For details, see *http://arweb.sdsu.edu/es/registrar/schedule_adjustment.html* (Links to an external site.)

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 I cannot provide accommodations based upon disability until I have received an accommodation letter from Student Disability Services. Your cooperation is appreciated.

Final: Wednesday, Dec. 14, 2021 8:00 – 10:00 AM. Be sure to plan accordingly.

The following schedule is tentative. The lecture days for each secion may vary during the course of the semester. The schedule will be updated as the semester progresses.

	Mon	**Wed**	**Fri**
Aug. 22	Introduction; Prologue Lab 0 Introduction to Excel	Prologue Lab 0 Introduction to Excel	Prologue
Aug. 29	Focus 7B,C Lab 1 Intro to Excel (cont.)	Focus 7B,C Lab 1 Intro to Excel (cont.)	Ch. 7B,C
Sept 5	**Labor Day**	Focus 7B,C No lab	Focus 7D,E,F
Sept 12	Focus 7D,E,F Lab 2 Numerical Int	Focus 7D,E,F Lab 2 Numerical Int	**Exam I**
Sept 19	Focus 7D,E,F Lab 3 UV-Visible/Error	Focus 7D,E,F Lab 3 UV-Visible/Error	Focus 8
Sept 26	Focus 8 Lab 4 Instrumental noise	Focus 8 Lab 4 Instrumental noise	Focus 8
Oct 3	Focus 8 Lab 5 Error propagation	Focus 8 Lab 5 Error propagation	Focus 9
Oct 10	Focus 9 Lab 6 Linear fit-1	**Exam II** Lab 6 Linear fit-1	Focus 9
Oct 17	Focus 9 Lab 7 Nonlinear fit-1	Focus 10 Lab 7 Nonlinear fit-1	Focus 10
Oct 24	Focus 10 Lab 8 Nonlinear fit-2	Focus 10 Lab 8 Nonlinear fit-2	Focus 10
Nov 31	Focus 11A,B Lab 9 Linear fit-2	Focus 11A,B Lab 9 Linear fit-2	Focus 11A,B
Nov 7	Focus 11 C,D Lab 10 Gaussian program	**Exam III** Lab 10 Gaussian program	Focus 11C,D
Nov 14	Focus 11C,D Lab 11 Potential energy curves	Focus 11F,G Lab 11 Potential energy curves	Focus 11F,G
Nov 21	Focus 11F,G	Thanksgiving Break	Thanksgiving Break
Nov 28	Focus 12A,B	Focus 12A,B	Focus 12A,,B
Dec 5	Focus 12A,B	Focus 12A,B; review **Last day of class**	
Dec 12		**Final: Wednesday, Dec. 14, 2022, 8:00 – 10:00 AM**	