CHEM 1410: Quantum Chemistry and Spectroscopy

Fall 2019

At a Glance

Course Meetings TuTh 1-2:15pm in Chevron 150

Recitation W 2-2:50pm in Chevron 150

Professor Jennifer Laaser
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Teaching Assistant Zijian Huo
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Office Hours Dr. Laaser: F 11am-noon in Chevron G12A

Zi: M 10am-11am on the 2nd floor balcony

Prerequisities The prerequisites for this course are:

- Two semesters of general chemistry (CHEM 0110 & 0120 or equivalent)
- Two semesters of introductory physics (PHYS 0174 & 0175 or equivalent)
- Math through calc 3 (MATH 0240 or CHEM 1000 or equivalent)

If you are uncertain about whether your preparation is sufficient for this course, please don't hesitate to ask.

Required Materials The following workbook is required for this course:

Quantum Chemistry and Spectroscopy: A Guided Inquiry
Tricia D. Shepherd & Alexander Grushow
2nd edition (2019)

This workbook is available as a Course Pack from the University Store for $25. You MUST purchase the version available from the University store; it is not the same as the version sold on Amazon.

Each student will also need a scientific or graphing calculator for use on in-class activities and exams.

Additional Recommended Materials While not required, you may also find the following two texts useful references:

Quantum Chemistry and Spectroscopy
Thomas Engel
4th edition (2019)

Applied Mathematics for Physical Chemistry
J. Barrante
3rd edition (2016)

Course Goals

Overview Chem 1410 is an introductory course in quantum mechanics and spectroscopy. My goal in this course is to help students develop a strong conceptual and mathematical understanding of the foundations of quantum mechanics and their implications in chemical systems.

Key Concepts By the end of the course, students will be able to:

- Explain the need for quantum mechanics in describing physical systems
- Articulate the postulates of quantum mechanics and apply them to model problems
- Use quantum mechanics to quantitatively describe the structure of atoms and molecules
- Discuss the quantum mechanical basis for vibrational, rotational, and atomic/electronic spectroscopies
- Explain how the basic quantum mechanical concepts explored in this course form the basis of modern methods in computational chemistry

Detailed lists of learning objectives will be posted on CourseWeb for each major unit of the course.

Course Structure

Grading Your "base grade" in this course will be determined by your scores the following items:

Item	Points Possible
Problem Sets (10 points each)	100 points
Midterms (100 points each)	200 points
Final Exam	150 points
Participation	50 points
Total	500 points

Final grades will be determined using the percent of total points earned. Nominally, students earning 90-100% of the points will earn A-range grades, students earning 80-90% of the points will earn B-range grades, etc.; the instructor will never make these ranges narrower (i.e. curve grades down), but may make them wider (i.e. curve grades up) as necessary to compensate for overly difficult exams and assignments.

Additionally, as described below, you will have the opportunity to bump your grade up one rung (i.e. from an A to an A+, or from a B- to a B, etc.) by completing challenge problems that push beyond the core course material.

Homework Problem sets will be assigned approximately once a week, and will be due by the start of class one week after they are assigned. There will be 10 problem sets over the course of the semester, each worth 10 points.

To receive full credit for your homework assignments, you must:

[1] Show *all* of your work, including all steps in manipulating equations, inserting numerical values, and evaluating the results
[2] Clearly organize and present your work, with enough written text/narrative to make it clear what you are doing and why
[3] Include units in all steps of numerical calculations, give answers with a reasonable number of significant figures, and use correct scientific notation

[4] For problems with Excel spreadsheets used for repetitive calculations, write out one calculation in full, and include a printout or screenshot of the spreadsheet when submitting your assignment

Finally, to facilitate efficient marking and return of submitted work, we will use Gradescope for submission and grading of problem sets and exams. If you are officially registered for this class, you should receive an invitation to Gradescope within 24 hours of the first class meeting; if you are auditing and are not officially registered, please contact the instructor for access. If you are unable to submit your work online due to technical problems, you should email a copy of your completed work to the instructor before the start of class, or, if absolutely necessary, may bring a hard copy to turn in in class. Solutions will be posted online shortly after the due date, and as such, no credit will be given for problem sets turned in after the class in which they are due.

You may *discuss* homework problems with your fellow students, but each student must prepare their own solutions independently.

Challenge Problems

Alongside the required problem sets, the instructor will assign 10 *optional* challenge problems that push beyond the core material for the course. These challenge problems will typically require more mathematical sophistication and/or deeper physical insight than regular homework problems. You *may not* work with other students to complete the challenge problems.

Challenge problems will be graded on an E/M/P/X scale, where "E" and "M" denote substantial mastery of the problem, with no ("E") or only minor ("M") mistakes; "P" denotes some progress but an incomplete solution; and "X" denotes no significant progress. If you complete at least 8 challenge problems with at least a "P", and at least 5 of those with at least an "M", Dr. Laaser will bump your grade up one rung (i.e. from an A to an A+, or from a B- to a B, etc.) at the end of the semester.

Note that these problems are intended to offer an extra challenge for students who are particularly interested in physical chemistry, but they are *completely optional*. You can earn an A in this course solely based on your performance on problem sets, exams, and your in-class participation; the number of students who do or do not complete the challenge problems will not influence the way in which the homework, exams, and participation scores are curved.

Exams

Exams will be based on the material from the lectures and in-class activities and the problem sets. Midterms will be given during the normal class meeting times (see schedule, below), and the final exam will be given on the date listed on Pitt's official final exam schedule. More details on exam format and expectations will be provided as the exam dates approach.

Scores for midterms missed due to excused absences will be replaced by the student's score on the final exam; otherwise, missed midterm exams will be given a zero.

Participation

Course meetings will consist of a mix of lectures and in-class activities, through which you will explore the core concepts for this class. These activities will be conducted in small groups, which will be assigned by the instructor at the start of each unit.

To encourage your regular attendance and participation, you will receive a small number of points for each class period in which you are in class *and* actively participating in the in-class activities with your group. You will not receive participation points for classes you miss unless except in the case of conflicts with religious observances, documented illness or a personal or family emergency (see make-up policy, below).

Recitations will generally consist of activities intended to help you develop your quantitative problem-solving skills. Attendance at recitation is strongly encouraged, but will generally not be counted toward participation scores. In a few cases, recitations

will be used to continue lectures and/or activities from the course meetings; when applicable, the instructor will announce this at the end of the preceding lecture period, and students will be expected to attend recitation to receive full participation credit for the week.

Schedule

Important Dates Class will meet regularly on Tuesdays and Thursdays at 1:00pm, and recitation will meet on Wednesdays at 2:00pm, with the following exceptions:

August 27	First day of class
October 3	Midterm 1 *(tentative)*
November 7	Midterm 2 *(tentative)*
November 26-28	No class or recitation - Thanksgiving break
December 5	Last day of class
December 12	Final exam (2pm-3:50pm, location TBD)

Please note that exam dates are *tentative* and are subject to change; finalized exam dates will be announced as soon as they are scheduled, and in all cases no later than one week before the exam.

Other Policies

Office Hours If you are unable to attend regularly scheduled office hours, please send an email to set up an individual meeting. Please note that these meetings are *by appointment only*, and must be scheduled at least 24 hours in advance.

Email Prof. Laaser will make an effort to respond to all course-related emails within 24 hours on weekdays and 48 hours on weekends.

If you have a more immediate question, especially about the homework problems, you are encouraged to discuss it with your TA and/or your fellow students, either in person or via the course discussion forums on CourseWeb/Blackboard.

Classroom Environment I strongly believe in the importance of the diversity of views, experiences, and identities of those in our scientific community. It is my goal that students from all backgrounds and perspectives be welcomed and well-served by this course. If there are aspects of the design, instruction, and/or your experiences within this course that you feel are acting as barriers to your full participation or achievement, please let me know as soon as possible so that we may take steps to address them.

Classroom Recording To ensure the free and open discussion of ideas, students may not record classroom lectures, discussion and/or activities without the advance written permission of the instructor, and any such recording properly approved in advance can be used solely for the student's own private use. If you have (or think you may have) a disability such that you need to record or tape classroom activities, you should contact your instructor and the Office of Disability Resources and Services (see below) to request an appropriate accommodation.

Academic Integrity Students in this course will be expected to comply with the University of Pittsburgh's Policy on Academic Integrity (http://www.cfo.pitt.edu/policies/policy/02/02-03-02.html). Any student suspected of violating this obligation for any reason during the semester will be required to participate in the procedural process, initiated at the instructor level, as outlined in the University Guidelines on Academic Integrity. This may include, but is not limited to, the confiscation of the examination of any individual suspected of violating University Policy. Furthermore, no student may bring any

unauthorized materials to an exam, including dictionaries and programmable calculators.

Disabilities If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact both your instructor and the Office of Disability Resources and Services (http://www.drs.pitt.edu/), 140 William Pitt Union, (412) 648-7890, drsrecep@pitt.edu, (412) 228-5347 for P3 ASL users, as early as possible in the term. DRS will verify your disability and determine reasonable accommodations for this course.

Absences & Make-Up Policy If you must miss a required class activity or exam for any reason, please contact me as soon as possible so that we can make alternate arrangements.

While some exceptions may apply, make-up work will generally only be offered in the case of conflicts with religious observances, documented illnesses, and personal or family emergencies.