

# Physical Chemistry 1: Quantum Chemistry & Spectroscopy

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**Web:** [canvas.pitt.edu](https://canvas.pitt.edu) + [piazza.com/pitt/fall2025/chem1410](https://piazza.com/pitt/fall2025/chem1410)

**Office Hours:** TBD

(or e-mail for an appointment)

**Meetings:** M, W 6-7:10 PM 228 Eberly Hall

**Textbook:** T. Engel, *Physical Chemistry: Quantum Chemistry and Spectroscopy*, 4<sup>th</sup> ed; 2018

**Required:** Scientific calculator with at least functions for: sin, cos, tan, exp, log,  $x^y$ , and  $\sqrt{x}$

**Optional Text:** J. Straub, *Mathematical Methods in Molecular Science*

**Course Goals:** To introduce you to quantum mechanics, including bonding and spectroscopy. This includes: particles, waves, Schrodinger's equation, postulates of quantum mechanics, applications of quantum models, bonding, vibrational, rotational, and molecular spectroscopy.

## Grading:

**Midterm Exams:** 25%

**Group Project:** 25%

**Final Exam:** 25%

**Homework:** 10%

**In-Class Quizzes:** 10%

**Piazza (discussion):** 5%

**Exams:** There will be two in-class midterms during the term. Each will be scheduled for the normal class period (70 minutes). The final is currently scheduled for **Monday, Dec 8th**. (We might do that as a take-home TBD.) Each exam will focus on material covered after the previous exam. More details on coverage will be outlined in class before the exam.

**Notes:** You will be allowed to bring ONE single-sided 8.5x11" sheet of paper with constants, parameters, equations, ... whatever you feel will help in the exam. No make-up exams will be given. If the failure to take an exam is due to a serious illness or emergency, then the grade will be averaged appropriately.

**Homework & Quizzes** To aid in the study of the course material, you will be given regular assignments (roughly one every two weeks). The assignments will be graded and returned before exams. Other weeks will include 10-minute quizzes — you can consider these as focusing on key ideas (i.e., not math speed).

**Piazza** Discussion is important and will help you understand the material. Regular polls, questions, and discussion are expected on the Piazza forum. To encourage good questions (and answers), participation will count for a small part of your grade.

This is the **International Year of Quantum** [quantum2025.org](https://quantum2025.org) so you can also gain extra credit by posting unique articles about quantum science and technology (journal articles, news, etc.) from reputable sources.

## Projects

As noted above, and on the syllabus schedule, one evaluation in the course will be a group project in quantum / computational chemistry "in real life." Groups of 3-5 students will select topics, perform quantum chemical calculations, and prepare videos for presentation, kudos, and possibly Internet glory. (Glory not guaranteed.)

**Disability Services**

If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact both your instructor and [Disability Resources and Services \(DRS\)](#), 140 William Pitt Union, (412) 648-7890, [drsrecep@pitt.edu](mailto: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.

**Title IX:**

“No person in the United States shall, on the basis of sex, be excluded from participation in, be denied the benefits of, or be subjected to discrimination under any education program or activity receiving Federal financial assistance.”

As a professor I am a mandatory reporter, and I am required to report violations of Title IX that I observe or am made aware of to the Title IX office (<https://www.titleix.pitt.edu/>). Title IX violations include, but are not limited to, sexual harassment, sexual violence and verbal or sexual abuse. Within the classroom, behavior in violation might appear as: suggestive jokes or innuendos, inappropriate touching, and unwanted sexual behavior or advances, but my obligation to report does not end at the classroom.

***Inclusion:*** We support an inclusive and open learning environment in which individual differences and opinions are understood, respected, and appreciated. We expect that students, TAs, and faculty will promote an atmosphere of respect for all members of the class. Expressions or actions that disparage a person's race, ethnicity, nationality, political opinions, culture, gender, gender identity / expression, religion, sexual orientation, age, disability, or marital, parental, or veteran status are contrary to the mission of this course and will not be tolerated.

If you encounter any issue, with other students or the TA, please contact the instructor. For an incident involving the instructor, please contact the Department of Chemistry and the Dietrich School's Ombuds office.

**Your Well-being Matters**

College can be an exciting and challenging time for students. Taking time to maintain your well-being and seek support can help you achieve your goals and lead a fulfilling life. It can be helpful to remember that we all benefit from assistance and guidance at times, and there are many resources available at Pitt. Visit [Thrive@Pitt](#) to learn more about well-being and the many campus resources available.

If you or anyone you know experiences overwhelming academic stress, persistent difficult feelings and/or challenging life events, you are strongly encouraged to seek support. In addition to reaching out to friends and loved ones, consider connecting with a faculty member you trust for assistance connecting to helpful resources.

The [University Counseling Center](#) is also here for you. You can call 412-648-7930 at any time to connect with a clinician. If you or someone you know is feeling suicidal, please call the University Counseling Center at any time at 412-648-7930. You can also contact Resolve Crisis Network at 888-796-8226. If the situation is life threatening, call Pitt Police at 412-624-2121 or dial 911.

**Academic Integrity**

Students in this course will be expected to comply with the University of Pittsburgh's [Policy on Academic Integrity](#). 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.

To learn more about Academic Integrity, visit the [Academic Integrity Guide](#) for an overview of the topic. For hands-on practice, complete the [Understanding and Avoiding Plagiarism tutorial](#).

**AI / ML Usage**

I am well aware of use and capabilities of current AI models, such as ChatGPT, Claude, Gemini, etc. We will talk about what works and what does not during the class. Spoiler - setting aside the lack of capabilities to perform math correctly, much less chemical knowledge, it is unethical to use AI models to perform your work. (Would it be ethical to have a friend do your work?)

My expectation is that while students will work together, discuss course material themselves, on Piazza, in office hours, etc. your graded homework and exams is your work alone.

# Physical Chemistry 1

## Topics and Readings

The schedule is tentative, although every effort will be made to stay on schedule

Topic	Date	Reading	HW / Quiz
Introduction & Review of Classical Physics	8/25		
Problems with Classical Physics	8/27	Ch. 1	
<b>LABOR DAY</b>	9/1		
Schrödinger's Equation & Waves	9/3	Ch. 2	
QM Postulates & Particle in a Box	9/8	Ch. 3 & 4	Quiz 1
Particle in a Box (cont.)	9/10	Ch. 4	
Particle in a Finite Box	9/15	Ch. 5	HW 1 Due
Applications (Tunneling, Nanoparticles, etc.)	9/17	Ch. 5	
Heisenberg Uncertainty, Entanglement, <b>REVIEW</b>	9/22	6.1 - 6.3	Quiz 2
<b>EXAM #1</b>	9/24		
Vibrational Motion: Harmonic Oscillator	9/29	7.1, 7.3	
Rotational Motion in 2D & 3D	10/1	7.2, 7.4, 7.7	HW 2 Due
Hydrogen Atom	10/6	7.5	
Hydrogen Atom (cont.)	10/8	Ch. 9	Quiz 3
<b>REVIEW</b>	10/13		HW 3 Due
<b>EXAM #2</b>	10/15		
Many Electron Atoms & SCF	10/20	Ch. 10	
Chemical Bonding & Molecular Orbitals	10/22	Ch. 12	Quiz 4
Bonding & Molecular Electronic Structure	10/27	Ch. 13	
Computational Chemistry	10/29	Ch. 15	HW 4 Due
Computational Chemistry (cont)	11/3		
Molecular Symmetry	11/5	Ch. 16	Quiz 5
Atomic Spectroscopy	11/10	Ch. 11	
Diatomic Vibrations & Rotations	11/12	Ch. 8	HW 5 Due
Electronic Spectroscopy	11/17	Ch. 14	
NMR Spectroscopy	11/19		
<b>THANKSGIVING BREAK</b>	11/24		
<b>THANKSGIVING BREAK</b>	11/26		
Video Projects	12/1		HW 6 Due
Review	12/3		Quiz 6
<b>FINAL EXAM</b>	<b>12/8</b>		