Syllabus for CHM 432: Physical Chemistry II

Spring 2024

Instructor Information

Instructor	Email	Office
Prof. Daniel Thomas	dathomas@uri.edu	474D Beaupre Center

Office Hours and Contact

Tuesdays, 11:00 AM – 12:00 PM
Wednesdays, 11:00 AM – 12:00 PM
Beaupre 474D

You are also welcome to set up an appointment. If you send me an email after 6 PM, I likely will not be able to respond until the next day.

On Brightspace, there will be a discussion forum where you can submit questions. The advantage of submitting a question here is that other students may have the same questions as you, so we can all learn together. If you wish, your name in these posts can be hidden from other students (although I can still see the post author).

General Information

Description

This course seeks to provide an overview of fundamental concepts in physical chemistry that will assist you in your future education or career. The main learning topic in this course is quantum chemistry, which we be the focus of >80% of the semester. We will explore the wave nature of matter and how this gives rise to the atomic and molecular properties that you have been learning since general chemistry. We will also discuss the experimental methods that support this description of atoms and molecules. The final portion of the course will provide a brief discussion of chemical kinetics, including the kinetic theory of gases, transition state theory, and the origin of reaction rate laws.

The intention of this course is not to test your mathematical aptitude. However, we will employ algebra and basic calculus throughout the course to gain chemical insight. Because we don't have time to cover all mathematical topics in detail, this course must rely on your prior mathematical knowledge. For topics that you may not have seen before, such as solutions to differential equations or linear algebra, the course will provide an overview of methods. If you find you are struggling with the math, please speak with me.

The strong emphasis on mathematical (especially calculus-based) approaches can be a tough transition from other courses in chemistry, so I ask for empathy, understanding, and flexibility as we navigate this course together. I am always open to changing the way the course is run if you find it isn't working. A list of planned course topics is given in the course schedule below.

Learning Objectives

At the end of the course, you will be able to…

- solve the time-independent Schrödinger equation for idealized systems and interpret the resulting solutions.

- relate the reactivity, structure, and properties of atoms and molecules to the underlying quantum chemistry.
- describe fundamental spectroscopic techniques in experimental physical chemistry and how they can be utilized to assess molecular structure, properties, and reaction dynamics.
- explain the relationship between the behavior of individual atoms or molecules and the overall properties of an ideal system (for example an ideal gas or a basic chemical reaction).

Website

All course materials and information will be posted to the course Brightspace page.

Course Meetings

All course meetings will take place weekly on Monday, Wednesday, and Friday from 10:00 AM to 10:50 AM. Although not anticipated, instructor illness may require the course to be taught online.

Course Structure, Course Philosophy, and Coursework

As in all other courses, you will learn the material best when you are actively engaged (meaning you are thinking hard about the content, not passively absorbing notes). However, you will need some background to tackle the relevant questions. Therefore, the course is structured to provide you with a mixture of introduction to topics and opportunities for hands-on practice.

Each week, we will go over concepts and work practice problems in class. Course notes will generally be posted to the Brightspace page for your reference, but looking at these notes is absolutely not a substitute for attending class. Class attendance is essential for succeeding in this course.

On Fridays, there will be an in-class assignment that will be due at the end of class (with a grace period until Monday). These assignments will be designed to be completed in 20–30 minutes.

To provide further practice, a problem set will be posted to the Brightspace page each week. These problem sets will not be submitted for a grade. However, it is essential that you work these problems to develop competence with the course material.

To incentivize keeping up with the material (and make sure that your work is reflected in your grade), there will be an online "quiz" for each week. The quiz does not have a time limit and can be accessed multiple times, but it can only be submitted once. The quiz will be due on Monday evenings with a 48-hour grace period.

There will be three exams throughout the semester, tentatively scheduled for Friday, February 16; Friday, March 22; and Friday, April 19. Exam dates are subject to change. Your most valuable tool in preparing for the exams will be the problem sets.

The final exam will take place on Friday, May 3 from 8:00 to 10:00 AM.

Software

This course will possibly use Zoom. It can be run in a browser or as a desktop application. Once you have your URI credentials, you will be able to log in at uri-edu.zoom.us.

Although not required for the course, there will be interactives notes posted that use the program Mathematica. Mathematica is an integrated tool where one can perform mathematical calculations, write code, interact with demonstrations, and visualize data. It's a very useful tool! To obtain a free license for Mathematica you can navigate to https://www.math.uri.edu/mathematica/. From there, you will directed to the Wolfram website, where you can log in with your URI credentials and download Mathematica. More detailed instructions are available in the "Start Here" module of the Brightspace page.

Course Grading

Methodology

Please try to keep in mind that your mastery of the course learning objectives is far more important than the letter or number grade you receive. I know that can be challenging, but try to ask yourself primarily if you are meeting each week's learning objectives.

Grade Breakdown

Your grade will be calculated based upon the following assignments:

- Online "quizzes" - 30% - these will be assigned weekly (except when there is an exam). You are welcome to work together in groups, but note that the response order and values may be different for each student. These quizzes will be due on Mondays at 11:59 PM via Brightspace. There is a grace period until 11:59 PM on Wednesdays. Your lowest quiz score will be dropped.
- In-class Assignments - 10% - this grade will come from submission of in-class assignments. Your lowest score will be dropped.
- Exams - 40% - there will be three in-class exams, tentatively scheduled for Friday, February 16; Friday, March 8; Friday, March 22; and Friday, April 19. Exam dates are subject to change.
- Final exam – 20% - this exam will take place on Friday, May 3 from 8:00 to 10:00 AM.

Grading Rubric

Unless otherwise noted, responses in all assignments will be evaluated according to the rubric below.

Category	Proficient	Emerging	Needs Improvement
Organization (Does response clearly show relevant information?)	Response is clear and easy to follow (1)	Information is not well-organized; some information is missing (0.5)	Clear path to solving problem is not explained; response does not include necessary elements (0)
Methods (Does answer show a clear plan with correct application of methods to achieve a reasonable solution?)	Takes the correct approach to arrive at the answer; for conceptual questions, the scope of the question is adequately addressed; logic leading to answer is clear; choices are justified; steps taken are included in equation or text form (6)	Takes a partially correct approach, but the method is oversimplified or insufficient; for conceptual questions, the response does not fully address the prompt; insufficient explanation is given; logic is sometimes hard to follow; steps in solving the problem are missing (3.5)	Takes an incorrect approach to the answer; approach to problem is not correct or appropriate; reasoning not supported by work shown; relationship of answer to prompt is not clear (1)
Results (Is the result accurate and complete?)	Solution is accurate and verified; algebraic or arithmetic errors are absent; proper references to concepts are included (3)	The response does not fully address the scope of the question, minor errors in analysis or arithmetic are present; evidence is missing for the result (1.5)	Very few or no steps are included; insufficient explanation for text responses or for the obtained answer (1)

Percent to Letter Grade

Final grades will be assigned on a basis not stricter than

A+, A, A− > 90% ; B+, B, B− > 80% ; C+, C, C− > 70 ; D+, D, D− > 60%

Course Materials

Required Text

Quantum Chemistry and Spectroscopy, Thomas Engel, Pearson, 2019, 4th Edition

Thermodynamics, Statistical Thermodynamics, and Kinetics, Thomas Engel and Philip Reid, Pearson, 2019, 4th Edition

Additional Resources

A Brief Review of Elementary Quantum Chemistry, C. David Sherrill, Georgia Tech, http://vergil.chemistry.gatech.edu/notes/quantrev/quantrev.pdf

Introduction to Statistical Mechanics, Peter Eastman, Stanford University, https://web.stanford.edu/~peastman/statmech/

Course Policies

Academic Honesty

Students are expected to be honest in all academic work. A student's name on any written work, quiz or exam shall be regarded as assurance that the work is the result of the student's own independent thought and study. Work should be stated in the student's own words, properly attributed to its source. Students have an obligation to know how to quote, paraphrase, summarize, cite and reference the work of others with integrity. The following are examples of academic dishonesty.

- Using solutions from another student or a previous semester to answer assignment questions
- Using material, directly or paraphrasing, from published sources (print or electronic) without appropriate citation
- Claiming disproportionate credit for work not done independently
- Unauthorized possession or access to exams or unauthorized communication during exams
- Unauthorized use of another's work or preparing work for another student
- Taking an exam for another student
- Altering or attempting to alter grades
- The use of notes or electronic devices to gain an unauthorized advantage during exams
- Fabricating or falsifying facts, data or references
- Facilitating or aiding another's academic dishonesty
- Submitting the same paper for more than one course without prior approval from the instructors.

Late Assignments and Extension Policy

Absences due to serious illness or traumatic loss, religious observances, or participation in a university sanctioned event are considered excused absences. Students are responsible for work missed during an excused absence but will not be penalized by grading or assignment/exam make-up policies. Students should notify me in advance of absences due to religious observance or university-sanctioned events and as soon as possible for other absences. See University Manual sections 8.51.11-8.51.14 for details.

Delays that fall outside of these categories are not considered acceptable reasons for missing class or turning in assignments late. If you are struggling to keep up with course material, please contact me. Because the quiz solutions are distributed at the end of the grace period, it is not possible to complete quizzes past this time except under extraordinary circumstances. Any late assignment will be subject to a penalty of 20% per day (one day late: 80% maximum grade, two days late: 60% maximum grade, etc.).

Viral Illness Precaution Statement

The University is committed to delivering its educational mission while protecting the health and safety of our community. Students who are experiencing symptoms of viral illness should NOT go to class/work. Those who test positive for COVID-19 should follow the isolation guidelines from the Rhode Island Department of Health and CDC.

If you are unable to attend class, please notify me prior to the start of class at dathomas@uri.edu.

Anti-Bias Statement

We respect the rights and dignity of each individual and group. We reject prejudice and intolerance, and we work to understand differences. We believe that equity and inclusion are critical components for campus community members to thrive. If you are a target or a witness of a bias incident, you are encouraged to submit a report to the URI Bias Response Team at www.uri.edu/brt. There you will also find people and resources to help.

Mental Health and Wellness

I understand that attending university comes with challenges and stress associated with your courses, job/family responsibilities, and personal life. URI offers students a range of services to support your mental health and wellbeing, including the URI Counseling Center, MySSP (Student Support Program) App, the Wellness Resource Center, and Well-being Coaching.

Disability Services for Students

Your access in this course is important. Please send me your Disability, Access, and Inclusion (DAI) accommodation letter early in the semester so that we have adequate time to discuss and arrange your approved academic accommodations. If you have not yet established services through DAI, please contact them to engage in a confidential conversation about the process for requesting reasonable accommodations in the classroom. DAI can be reached by calling: 401-874-2098, visiting: web.uri.edu/disability, or emailing: dai@etal.uri.edu.

Land Acknowledgement

The University of Rhode Island land acknowledgment is a statement written by members of the University community in close partnership with members of the Narragansett Tribe. The statement recognizes and pays tribute to the people who lived on and stewarded the land on which the University now resides. The statement seeks to show gratitude and respect to Indigenous people and cultures and build community with the Narragansett Nation and other Native American tribes.

University of Rhode Island Land Acknowledgment

The University of Rhode Island occupies the traditional stomping ground of the Narragansett Nation and the Niantic People. We honor and respect the enduring and continuing relationship between the Indigenous people and this land by teaching and learning more about their history and present-day communities, and by becoming stewards of the land we, too, inhabit.

Course Schedule

Week	Topic	Book Chapter	Notes
Week 1 (Jan. 22-27)	The Quantum Nature of Matter, Heisenberg Uncertainty Principle	1, 6.3	Prior Knowledge Quiz Due
Week 2 (Jan. 28- Feb.3)	Wave Equation, Time-Independent Schrödinger Equation	2	Week 1 Quiz Due

Week	Topic	Book Chapter	Notes
Week 3 (Feb. 4-10)	Postulates of QM, Particle in a Box, Entanglement	3, 4	Week 2 Quiz Due
Week 4 (Feb. 11-17)	Hydrogen Atom	9	Week 3 Quiz Due, Exam 1
Week 5 (Feb. 18-24)	Multielectron Atoms	10	No Quiz, No Class on Monday
Week 6 (Feb. 25- Mar. 2)	Atomic Spectroscopy	11	Week 5 Quiz Due
Week 7 (Mar. 3-8)	Chemical Bonding	12	Week 6 Quiz Due
Week 8 (Mar. 17-23)	Vibrational and Rotational Motion	7	Week 7 Quiz Due, Exam 2
Week 9 (Mar. 24-30)	Vibrational and Rotational Spectroscopy	8	No Quiz
Week 10 (Mar. 31-Apr. 6)	Molecular Electronic Spectroscopy	14	Week 9 Quiz Due
Week 11 (Apr. 7-13)	Kinetic Theory	16, 17	Week 10 Quiz Due
Week 12 (Apr. 14-20)	Chemical Kinetics	18	Week 11 Quiz Due, Exam 3
Week 13 (Apr. 21-27)	Statistical Mechanics		No Quiz
Week 14 (Apr. 28- May 4)	Exam Prep		Week 13 Quiz Due Final Exam