Syllabus for CHM 507: Chemical Structure and Material Properties

Fall 2020

Instructor Information

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

Office Hours

Tuesdays, 9–10 AM
Wednesdays, 1–2 PM
Via Zoom
You are also welcome to set up an appointment.
Additionally, you can send me questions via email. If you send me an email after 6 PM, I likely will not be able to respond until the next day. There will also be a discussion forum where you can ask questions.

General Information

Description

This course seeks to provide an overview of fundamental concepts in physical chemistry that you will assist you in your graduate career. The primary goals of the course are both to promote basic skills in physical chemistry and to provide tools that will be directly useful to you as a researcher.

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. As we don't have time to cover all mathematical topics in detail, this course has to rely on your prior mathematical knowledge. For some topics, such as linear algebra, the course will provide an overview of methods. If you find you are struggling with the math, please speak with me.

This semester will certainly be anomalous in many ways, so I ask for empathy, understanding, and flexibility as we navigate this course together. We may have to change the format if we 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…

- recognize the nomenclature, concepts, and methods related to quantum chemistry and statistical mechanics that often appear in the research literature.
- relate the reactivity, structure, and properties of molecules to the underlying quantum chemistry.
- select appropriate electronic structure methods to predict the structures and properties of molecules.
- describe common techniques in experimental physical chemistry and how they can be utilized to assess molecular structure, properties, and reaction dynamics.
- apply statistical mechanics to explain how the properties of a system, described by thermodynamic equations, arise from the behavior of individual molecules.

Website

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

Synchronous Meetings

Given the current pandemic situation, the course will be run entirely online, with synchronous sessions occurring on Monday, Wednesday, and Friday at 11 AM via Zoom.

Software

This course will utilize 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.

The course will also use 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 for your careers as researchers, and I would like to use it throughout the course. To obtain a free license for Mathematica you can follow the instructions at https://www.math.uri.edu/mathematica/ under How to Get Mathematica -> Students.

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:

- Problem sets - 40% - these will be assigned weekly and will be the most important opportunity for you to practice with the course material. You are welcome to work together in groups, but the work you turn in must be your own (i. e., please don't simply copy down answers from someone else).
- Pre-class quizzes - 10% - there will be one short quiz each week that must be completed by Sunday at 11:59 PM. The quizzes will cover content in the lesson videos. There will be a reflection question on each quiz that asks what is most challenging or confusing about this content, and we will use these responses to inform the synchronous discussion.
- Take-home exams - 40% - there will be two take-home exams, one in week 7 and one as the final exam to assess comprehension of the material. In contrast to the problem sets, these will not be collaborative assignments (meaning you must do the work alone). The second take-home exam will count as your final exam and will be due on Friday, Dec. 18 at 11 AM. Please check out the final exam schedule to see when your other course exams will be due and plan accordingly.
- Discussion - 10% - this will come from participation in the weekly discussion forums and from synchronous session participation. To receive participation credit, you must post a question or an answer to a question in the weekly discussion forum on Brightspace. To receive full discussion credit, you must post in at least 10 out of the 14 discussion forums (one for each week).

Percent to Letter Grade

Final grades will be assigned on basis not stricter than

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

Course Materials

Required Text

Physical Chemistry: A Molecular Approach, D. A. McQuarrie and J. D. Simon, University Science Books

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

COVID-19 Precautions and Policies

The University is committed to delivering its educational mission while protecting the health and safety of our students. At this uncertain time, those concerns include minimizing the potential spread of COVID-19 within our community. While the university has worked this summer to create a healthy learning environment for all, it is up to all of us to ensure our campus stays that way.

As members of the URI community, students are required to comply with standards of conduct and take precautions to keep themselves and others safe. Students are required to comply with Rhode Island state laws, including the Rhode Island Executive Orders related to health and safety, ordinances, regulations, and guidance adopted by the University as it relates to public health crises, such as COVID-19.

An addendum on policies and guidelines concerning your obligations during this crisis has recently been integrated into the Student Handbook. These obligations include:

- Wearing of face masks by all community members when on a URI campus in the presence of others
- Maintaining physical distancing of at least six feet at all times
- Following state rules on the number of individuals allowed in a group gathering
- Completing a daily health self-assessment also available through the Rhody Connect app before coming to campus
- Submitting to COVID-19 testing as the University monitors the health of our community
- Following the University's quarantine and isolation requirements

If you answer yes to any of the questions on the daily health assessment, do not come to class. YOU MUST STAY HOME and notify URI Health Services via phone at 401-874-2246 immediately.

If you are already on campus and start to feel ill, you need to remove yourself from the public and notify URI Health Services via phone immediately at 401-874-2246 and go home and self-isolate while you await direction from Health Services.

If you are unable to attend class, please notify me. We will work together to ensure that course instruction and work is completed for the semester.

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.

Disability Services for Students

Your access in this course is important. Please send me your Disability Services for Students (DSS) 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 DSS, please contact them to engage in a confidential conversation about the process for requesting reasonable accommodations in the classroom. DSS can be reached by calling: 401-874-2098, visiting: web.uri.edu/disability, or emailing: dss@etal.uri.edu.

Land Acknowledgement

We acknowledge that we gather as the University of Rhode Island on the traditional land of the Niantic and Narragansett people in past and present, and honor with gratitude the land itself and the people who have stewarded it throughout the generations. This calls us to commit to continuing to learn how to be better stewards of the land we inhabit as well.

Late Assignments and Extension Policy

If serious illness, accident, personal tragedy, or other serious matters prevent you from attending classes, taking examinations, or meeting deadlines, please contact me as soon as possible to make arrangements. 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. Late work will be subject to a deduction of 25% of the initial grade per day (i.e., one day late gives a maximum grade of 75/100, two days late a maximum grade of 50/100, etc.).

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 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.

Course Schedule

Week	Topic	Notes
Week 1 (Sep. 9–12)	Intro to QM, Complex Numbers, Fourier Series	Introduce Yourself
Week 2 (Sep. 13–19)	Fourier Transform, Heisenberg Uncertainty, Wave Equation, Time-Independent Schrödinger Equation	Week 2 Homework Due
Week 3 (Sep. 20–26)	Operators in QM, Postulates of QM, Harmonic Oscillator, Rigid Rotor	Week 3 Homework Due
Week 4 (Sep. 27–Oct. 3)	Hydrogen Atom, Multielectron Atoms	Week 4 Homework Due
Week 5 (Oct. 4–10)	Spin, Exchange, Hartree-Fock, Term Symbols, Hund's Rules	Week 5 Homework Due
Week 6 (Oct. 11–17)	Born-Oppenheimer Approximation, Molecular Orbitals, Valence Bond and Hybridization, Molecular Term Symbols	Week 6 Homework Due
Week 7 (Oct. 18–24)	Midterm Review, Computational Chemistry	Midterm Examination
Week 8 (Oct. 25–31)	Group Theory, Lasers and Spectroscopy	Week 8 Homework Due
Week 9 (Nov. 1–7)	Electronic Spectroscopy, NMR Spectroscopy	No Class Nov. 3, Week 9 Homework Due
Week 10 (Nov. 8–14)	Introduction to Stat Mech, Maxwell-Boltzmann Dist., Partition Function	No Class Nov. 11, Week 10 Homework Due
Week 11 (Nov. 15-21)	Thermodynamic Potentials and Forces, The Laws of Thermodynamics	Week 11 Homework Due
Week 12 (Nov. 22-28)	Heat and Entropy, Ideal Gas Law, Free Energy	Thanksgiving Break, Week 12 Homework Due
Week 13 (Nov. 29–Dec. 5)	Chemical Equilibrium and Chemical Kinetics	Week 13 Homework Due
Week 14 (Dec. 6–12)	Reaction Dynamics, Surface Chemistry	Week 14 Homework Due