Instructor: **Tyler Meldrum,** ISC 1060, 221-2561 *tkmeldrum@wm.edu*
Grader: Trinh Ton *tnton@wm.edu*

Course Meetings: Mondays, Wednesdays, Fridays 11:00–11:50 am, Tucker 127A
Thursdays 6:00–7:00 pm, ISC 1221 (review sessions held only before exams)

Instructor office hours: Tuesdays, 12:30–1:30 pm

Course Description
This course is intended for chemistry majors. In it, we will discuss principles and postulates of quantum mechanics and will develop simple quantum mechanical models that lead to an understanding of real molecules. We will review mathematical principles necessary to understand quantum mechanics, and we will discuss principles of atomic and molecular spectroscopy. Lastly, we will preview principles of chemical kinetics.

Text
Engel, T. Quantum Chemistry and Spectroscopy, 4th ed; Pearson: 2019. ISBN 978-0-13-480459-0.
This text is available to buy in print from the W&M Bookstore, Amazon, etc. for approximately $125/$75 (new/used). In addition, an eText is available directly from Pearson, access to which costs $45

Course Details
Blackboard site: This course makes extensive use of Blackboard. Please check the Blackboard site regularly for announcements, practice problems, lecture notes, grades, and other course supplements.

Gradescope: Grading in this course is done in Gradescope. Homework assignments will be uploaded to and graded in Gradescope. Exams will be done in class on paper, but will subsequently be scanned, uploaded to, and graded in Gradescope.

Lecture recordings: Barring major technical problems, I will be recording each lecture and posting it to Blackboard after each class period. Please use those recordings to help you study. Also, consider research that indicates that students who take notes by hand tend to outperform those who take notes on the computer. I suggest you focus on main concepts and their applications during lectures, then you can revisit the videos to catch any details that you may have missed.

Exams/quizzes: Three in-class exams will be given on **September 30, October 28, and December 2.** Each is worth 20% of the final grade. In addition, one quiz will be given before the first exam (available beginning September 16 and **due September 21**). The quiz is worth 10% of the final grade and is intended as a “warm up” to exams in physical chemistry. See grading notes below.

Final exam: A final exam will be given on **Tuesday, December 13 from 9:00 am–12:00 pm,** location to be announced (probably our regular lecture hall, Tucker 127A). The final exam will be worth 30% of the course grade and will be comprehensive. This time slot is assigned by the registrar and, with the few exceptions designated by the registrar, cannot be moved. Please notify me of any registrar-approved final exam exceptions well in advance.

Grading notes: I will drop 10% of your exam/quiz grades in your favor. This will be done automatically in one of the following ways (I’ll use whichever method maximizes your score):

1. **Drop the quiz score completely.** This will make the three exams collectively worth 60% of your grade and the final exam worth 30% of your grade. (90% total.)
2. **Reduce the value of the lowest exam score from 20% to 10% of the final course grade**. This will make two-and-a-half exams worth 50%, one quiz worth 10%, and the final exam worth 30% of your grade. (90% total.)
3. **Keep all exams and the quiz** (collectively 70% of your grade) **and make the final worth only 20% of your grade.** (90% total.)

Homework: Several homework assignments will be made throughout the semester. These will be approximately weekly with adjustments made for exam weeks and the pace of material. Collectively, the homework assignments will be worth 10% of the course grade. I encourage you to work on these assignments collaboratively. Each homework submission may come from between 1–4 people, with each member of that group receiving the same grade. You may but are not required to have the same homework groups throughout the semester.

This is a challenging, fast-paced course. I assign a lot of material because I want you to work with the content in smaller, more frequent pieces. I don't want you to slip behind. Please keep up with the material, know that the pace of the course is fast, and come see me if you feel like things are getting away from you.

Some important statements that I stand by.
Illness and absences: All lectures will be recorded and posted to Blackboard; please do not attend class if you are ill. If you are unable to take an exam due to illness, please inform the instructor as soon as possible, no later than 9 am the morning of the exam, to make accommodations. In addition, W&M students who test positive for COVID-19 need to isolate and not attend in-person classes for at least five days. Unvaccinated or un-boosted students also quarantine if they are identified as close contacts. Visit the CDC's Quarantine & Isolation Guide and Calculator for information.

Student Accessibility Services: William & Mary accommodates students with disabilities in accordance with federal laws and university policy. Any student who feels they may need an accommodation based on the impact of a learning, psychiatric, physical, or chronic health diagnosis should contact Student Accessibility Services staff at **757-221-2512** or at **sas@wm.edu** to determine if accommodations are warranted and to obtain an official letter of accommodation. For more information, please see **www.wm.edu/sas**.

Religious Accommodations: I am happy to accommodate holidays of organized religions. Please inform me by the end of the add/drop period of such observances that are likely to conflict directly with this class.

Honor Code: As members of the William & Mary community, we pledge on our honor not to lie, cheat, or steal, either in our academic or personal life. We understand that such acts violate the Honor Code and undermine the community of trust, of which we are all stewards.

Class Recordings: Meetings of this course will be recorded. Recordings will be available only to students registered for this class. This is intended to supplement the classroom experience. Students are expected to follow appropriate university policies and maintain the security of passwords used to access recorded lectures. Recordings may not be reproduced, shared with those not in the class, or uploaded to other online environments; violations may be subject to disciplinary action. If the instructor or a William & Mary office plan any other uses for the recordings, beyond this class, students identifiable in the recordings will be notified to request consent prior to such use.

Inclusivity: The Chemistry Department strives to create and maintain an inclusive environment for all our students, faculty, and staff. We want our classrooms, laboratories, and offices to be safe and welcoming places for all, regardless of how we may differ in age, cultural identity, ethnicity, gender, gender identity, faith, neurological make up (neurodiversity), geographic background, political and ideological perspectives, race, sexual orientation, and social and economic status. In addition, William & Mary values and actively nurtures an inclusive environment where every individual, regardless of race, religion, gender, ethnic origin, age, socioeconomic status, political preferences, physical abilities, or sexual orientation (a non-exclusive list) is respected and afforded the opportunity to grow and to succeed.

Physical Chemistry Course Learning Goals (adapted from CU Boulder)

1. *Foster intuition.* Develop an intuition about physical chemistry systems and models. This intuition may include:
   - Areas in which quantum and classical systems diverge.
   - The effects of quantization of energy.
   - Wave nature of matter and energy.
   - What operators do and how they work.
   - Ways in which energy may be manifest in atoms/molecules.
2. *Form connections between math and chemistry.* Translate a physical description of a physical chemistry problem into the mathematical formalism necessary to solve it. Explain the physical meaning of the mathematical formulation and solution. Develop physicochemical insight through the mathematics of a problem.
3. *Visualize.* Sketch appropriate parameters of a problem (e.g., wave function, potential, probability distribution). When presented with a graph of a wave function or probability density, derive appropriate physical parameters of a system.
4. *Predict, solve, and check problems.* As appropriate for a given problem, articulate expectations for the solution to a problem in advance of finding a complete solution, such as:
   - The general shape of the wave function.
   - Behavior at large/boundary distances.

   Learn to choose and apply appropriate problem-solving methods. Transfer the methods learned in class and through homework to novel contexts. Some specific problem-solving methods to be developed in this course include:
   - *Models.* Consider which physical chemistry models are most helpful when approaching a problem and implement them appropriately.
   - *Approximations.* Recognize when approximations are useful, and to use them effectively.
   - *Symmetry.* Recognize symmetry and be able to take advantage of it to solve a problem.
   - *Coordinate systems.* Recognize when using certain coordinate systems provide clear advantages for particular problems.

   Justify the reasonableness of a solution reached, by using methods such as:
   - Order of magnitude estimates.
   - Dimensional analysis.
   - Validating against limiting or special cases.
5. *Navigate the unknown.* Draw upon knowledge and skills to approach a problem even when a process leading to a correct solution is not yet clear. Develop the ability to monitor progress towards a solution by learning how to, among others:
   - Backtrack and try a new approach when necessary.
   - Recognize when a solution has been reached and be able to articulate why this solution is valid.
   - Persist through to the solution of problems requiring many steps.
6. *Develop intellectual maturity.* Students should accept responsibility for their own learning and be aware of what they do and do not understand about physical chemistry. Students should learn to ask specific questions, and to identify and articulate the parts of a problem that they found difficult so they can take appropriate action. Finally, students should regularly check their understanding against these learning goals and seek appropriate help to fill in gaps.

Tentative course schedule (as of 11 August 2022)—subject to change.

Dates	Topics	Text Sections
W, 8/31	Course introduction, math background	ME1, ME2, ME6
F, 9/2	Origins of QM	1.1–1.7
M, 9/5	*LABOR DAY—NO CLASS*	
W, 9/7	Boltzmann and quantization, the Schrödinger equation	2.1-2.3
F, 9/9	Operators, observables, eigenstuff *[Add/drop deadline]*	2.4–2.7
M, 9/12	Postulates, probability, normalization, expectation values	3.1–3.5
W, 9/14	Postulates, probability, normalization, expectation values continued	
F, 9/16	Free particle, particle-in-a-1D-box *(Quiz is available)*	4.1–4.2
M, 9/19	Particle-in-a-3D-box, degeneracy, PIB applications	4.3, 4.4, 5.3
W, 9/21	Commutators, Heisenberg uncertainty principle ***(Quiz due)***	6.1–6.4
F, 9/23	Molecular vibration: the harmonic oscillator	7.1, 7.3
M, 9/26	Molecular vibration: the anharmonic oscillator	8.3
W, 9/28	Vibrational spectroscopy	8.1–8.5
F, 9/30	***EXAM 1*** *(review session prior evening)*	
M, 10/3	Vibrational spectroscopy continued, selection rules	
W, 10/5	Molecular rotation: 2D rigid rotor; polar and spherical coordinates	7.2, 7.4, ME8
F, 10/7	Molecular rotation: 3D rigid rotor	7.5–7.8
M, 10/10	Rotational spectroscopy	8.1, 8.2, 8.4, 8.6
W, 10/12	Molecular rotation continued	
F, 10/14	*FALL BREAK—NO CLASS*	
M, 10/17	The hydrogen atom: formulation	9.1–9.3
W, 10/19	The hydrogen atom: visualization	9.4–9.6
F, 10/21	Determinants, the problem with multi-electron systems, electron spin	ME9, 10.1–10.3
M, 10/24	Variational method, Hartree-Fock self-consistent field	10.4–10.6
W, 10/26	Many-electron atoms, good quantum numbers, atomic term symbols	11.1–11.2
F, 10/28	***EXAM 2*** *(review session prior evening)*	
M, 10/31	Working with term symbols *[Withdraw deadline]*	
W, 11/2	Spin-orbit coupling, atomic spectroscopy	11.3–11.5
F, 11/4	Atomic spectroscopy continued	
M, 11/7	Molecular orbitals, Born-Oppenheimer, H_2^+, wavefunction symmetry	12.1–12.2
W, 11/9	MO theory continued	
F, 11/11	Energy of molecular orbitals	12.3–12.4
M, 11/14	Homonuclear diatomic orbital symmetry, multi-electron atomic configurations	12.5–12.6
W, 11/16	Electronic spectroscopy, molecular term symbols, diatomic transitions	14.1–14.3
F, 11/18	Electronic spectroscopy continued	
M, 11/21	Franck-Condon, vibrational structure of electronic transitions (pre-recorded)	14.4–14.5
11/23–25	*THANKSGIVING BREAK*	
M, 11/28	Fluorescence, phosphorescence	14.6–14.9
W, 11/30	Kinetic molecular theory, ideal gas law	ERT16.1–16.2*
F, 12/2	***EXAM 3*** *(review session prior evening)*	
M, 12/5	Maxwell-Boltzmann speed distribution	ERT16.3*
W, 12/7	Gas collisions, energy, and reactions	ERT16.6–16.7*
F, 12/9	No class meeting	
T, 12/13	***FINAL EXAM 9:00 am–12:00 pm***	

**ERT is Engel & Reid's Thermodynamics, the text you'll use next semester in CHEM 302. I will post relevant material on Blackboard.*