

**SYLLABUS - CHEM 352, PHYSICAL CHEMISTRY II, SPRING 2021****Tuesdays & Thursdays, 9:00-10:15 a.m. HST****Instructor:** Prof. Kristin K. Kumashiro**Email:** [kumashir@hawaii.edu](mailto:kumashir@hawaii.edu) (or send messages through Slack)**Office:** Bilger 241**Phone:** 956-5733 (campus office)**Required Text:** Physical Chemistry: A Molecular Approach, D. McQuarrie & J. Simon**Prerequisite:** **CHEM 351** (which required Calculus III and PHYS 170-272 as prerequisites)**Recommendations:** Minimum grades of "C" or better in 351, Calculus III **and** PHYS 170-272.

<b>Grading:</b>	Quiz, Exams 1-4	60%
	Final Exam, Tuesday, May 11, 2021, 9:45-11:45 a.m.	15%
	In-class activities, participation, attendance	15%
	<u>Problem Sets (Homework)</u>	<u>10%</u>
		<b>100%</b>

**Zoom Meeting Information:**

- All class meetings will be held on the Zoom platform. Use the [link](#) or

**Meeting ID:** [REDACTED] **(Passcode:** [REDACTED] **)**

- Your attendance is expected at all class meetings on Zoom, unless otherwise advised.
- Zoom attendance for all quizzes and exams is mandatory.

## TECHNOLOGY FOR CHEM 352 IN SPRING 2021

### ZOOM MEETING INFORMATION:

- All class meetings will be held on the Zoom platform. Use the [link](#) or  
**Meeting ID:** [REDACTED] **(Passcode:** [REDACTED])
- You received the Zoom invitation for the semester before the start of classes by email. A copy of the invitation is also posted to Laulima.
- Your attendance is expected at all class meetings on Zoom, unless otherwise advised.
- The lectures will be recorded and then posted to Laulima. If the chat is used, a copy of the transcript will also be posted.
- Zoom attendance for all quizzes and exams is mandatory.

### SOCRATIVE FOR IN-CLASS ACTIVITIES

- Socrative is used for in-class assessment. Your participation in the Socrative “quizzes” will count towards the “In-class activities” portion of your grade. It is also used to track attendance.
- Start by taking a look at the Socrative website (<https://www.socrative.com/>). You will enter through the student portal.
- Socrative Student is available as a (FREE) downloadable app in iOS, Chrome, and Google Play formats. (Use the student version, not the one for teachers.)
- You can decide between the app or the website (using your favorite browser).
- On your first login, you will be prompted for our Socrative “room”: [REDACTED]

### SLACK FOR OUT-OF-CLASS DISCUSSION AND QUESTIONS

- We are using the free version of Slack (<https://slack.com/>), which is supported on a number of platforms. You can also use Slack in your favorite browser.
- Use the Slack channels to ask questions, instead of Laulima or even email. Slack will allow everyone to see your questions & answers (from me or others, relevant discussion, etc,
- Use this [link](#) to join our Slack workspace ([REDACTED]). This link will expire on or about 2/3/2021. Please contact me for an updated invitation, if it expires before you are able to join.
- The Slack channels are akin to threads, and each is denoted with the hashtag. Please post your questions about the lab to the channel for 352 (# [REDACTED]).
- You are welcome to send DMs to Prof. Kumashiro via Slack.
- As always, write your messages with care and courtesy, and please treat each other (and me) in the respectful manner that you would use, if we were meeting in person.

## TENTATIVE SCHEDULE OF TOPICS

**STRUCTURE, PART I: INTRODUCTION, FOUNDATIONS, & ONE-DIMENSIONAL SYSTEMS.** This section will begin with lectures on the historical background of quantum mechanics. We will then study the Schrodinger equation and two one-dimensional models, particle in the box and the simple harmonic oscillator. Interwoven with the mathematical aspects of this material will be the postulates and general principles of quantum mechanics.

### WEEKS 1-2      HISTORICAL BACKGROUND      CHAPTER 1 (ALL SECTIONS)

This class begins with an overview of key developments in the early considerations of light and matter. Concepts related to waves and energy are reviewed. Topics include

- Blackbody radiation (ultraviolet catastrophe, Planck's hypothesis)
- Photoelectric effect.
- Bohr's model of the atom to explain line spectra in H atom.
- Heisenberg Uncertainty Principle. DeBroglie's wave-particle duality.

#### ASSESSMENT: QUIZ 1 (5%)

### WEEKS 3-5      THE SCHRODINGER EQUATION AND SIMPLE APPLICATIONS

#### POSTULATES & GENERAL PRINCIPLES OF QUANTUM MECHANICS

#### THE ONE-DIMENSIONAL PARTICLE IN A BOX

#### CH. 3-4 (EXCEPT 3.9)

This section begins with operators and operator algebra, as well as eigenfunctions and eigenvalues, all of which are essential to our discussion of quantum mechanics. Other important concepts include commutation (commuting operators).

After this introduction of (mostly) mathematical concepts and skills, the postulates of quantum mechanics are introduced. Key ideas include linear and Hermitian operators, Born interpretation (and well-behaved wavefunctions) and normalization, expectation values, orthogonality & orthonormality, and the significance of the commutator. Wave equations & the time-independent Schrodinger equation are also covered.

Then, the first model system (**one-dimensional particle in a box**) is discussed:

- Wavefunctions. Probability. Orthonormality.
- Energies and energy level diagram
- Expectation values.
- Butadiene example

#### ASSESSMENT: EXAM 1 (15%)

**WEEKS 6-8 THE HARMONIC OSCILLATOR**

5.1-5.7 &amp; 13\*

The **simple harmonic oscillator** is another one-dimensional system, for which the Schrodinger Equation is solved exactly. Lectures will cover:

- Review of classical picture.
- Schrodinger Equation, general expressions for the wavefunctions. Hermite polynomials. Tunneling.
- Energies of the harmonic oscillator.
- Morse potential for real molecules. Vibrational spectroscopy (\*selected sections of Ch. 13)

**ASSESSMENT: EXAM 2 (10%)**

**STRUCTURE, PART II: THREE-DIMENSIONAL SYSTEMS, APPROXIMATE METHODS, & ATOMS.** This section will begin with the two- and three-dimensional systems with exact solutions to the Schrodinger Equation, including the multi-dimensional particle-in-a-box, the rigid rotor, and the hydrogen atom.

**WEEK 9 PARTICLE IN A BOX IN 2 AND 3 DIMENSIONS****3.9**

Consider the **particle in a box** (covered in Ch. 3-4) in 2 and 3 dimensions. Key ideas include separation of variables. Note the relationships for energies (total energy) and wavefunctions (total wavefunction).

**WEEKS 10-11 RIGID ROTOR****MATHCHAPTER D, 5.8-5.9, 6.2-6.3, 13\***

This section begins with a review of Cartesian and spherical coordinate space. The Laplacian operator is defined in the different coordinate systems.

The first system to cover in spherical coordinate space is the "**particle on a ring**" (or **rotation in a plane**). We will discuss the Hamiltonian and its wavefunction.

Then, quantum mechanical picture of the **rigid rotor** (or "**particle on a sphere**") is described:

- Separation of variables to RR wavefunctions.
- Energies. Angular momentum.
- Rotational spectroscopy
- Rotational-vibrational spectroscopy

**ASSESSMENT: EXAM 3 (15%)**



## EXAMS AND QUIZZES

1. **Students with the privilege of attending the University of Hawai'i will conduct themselves honorably at all times. To give, to receive, or to use aid of any kind during an examination or quiz injures the university, students doing honest work, and the individual guilty of such dishonesty.** Acts of academic dishonesty include, but are not limited to, giving or receiving unauthorized assistance during an exam, obtaining unauthorized information about an exam before it is given, submitting another's work as one's own, using prohibited sources of information during an examination, and altering answers after an exam has been submitted. Such acts will result in the appropriate actions in accordance with the University of Hawaii's policy on student conduct and academic honesty.
2. **The exams (and one quiz) will include material from the lectures, reading assignments, and homework problems.** See previous pages for approximate schedule. Exam/quiz dates will be announced in class, roughly a week in advance. More details about the exam content will be given in class.
3. **Due to the nature of the current pandemic, exam procedures are under "ongoing consideration"**. Therefore, we may adopt additional exam-taking conditions, you may be given new exam-taking requirements, and/or existing policies may be modified.

I will do my best to keep you updated, so that we can all be prepared, with minimal anxiety about the procedures for each exam. As students, you will each need to be diligent in keeping up with what is happening in class.

4. **Exams will be administered online.** Exams will contain computer-graded questions (multiple-choice, fill-in-the-blank) and ones that I will grade (e.g., short answer, uploaded responses). Some problems will require a written response, which you will need to scan or capture and then upload it to Lulima.
5. **You are/will be advised on what items & resources you may use.** Some of the allowed items are listed here. **If an item or resource is not designated as "allowed", then its usage is prohibited.**
6. **You will be allowed to use a calculator for problems that include calculation.**
  - A calculator is a small electronic object designed specifically and solely for calculation.
  - Your calculator may be subject to a random check on the day of an exam.
  - Use of all other electronic devices are prohibited during the exams. You are not allowed to use the calculator function on your phone, tablet, smart watch, or any other mobile device.
  - You are not allowed to use the calculator app on your computer/laptop/etc.
  - You must clear the memory on your calculator before exams.
7. **Your cell phone may ONLY be used to scan and upload exam responses to Lulima. You may not use your cell phone for other purposes (texting, calls, etc.) during the exam.** If you expect an urgent call during the exam period, let me know BEFORE the class starts.
8. **Zoom attendance for all exams is mandatory.** Tentatively, video monitoring (via Zoom) will be implemented during the exams, which means that you will need to be working on a computer (or with a phone) that will have its camera facing you for the entirety of the exam.

9. **All exams are closed-book. However, for each exam, you will be allowed one index card (4" by 6") of your notes.** You can write whatever you want on it, and it should be prepared well in advance of the exam. It will not be collected or graded – it is solely for your use and benefit.
  10. **Please be ready to start on-time.** With the exception of the Final Exam (which starts at 9:45 a.m.), all exams will start at 9:00 a.m. HST
  11. **We'll use the entire class period for each exam.** The time limit for a quiz might be shortened, as less material is covered. No time extensions will be given to latecomers, except in unusual and exceptional circumstances.
  12. **If you miss (or will miss) an exam, you must let me know – as soon as possible – to discuss your absence.**
    - *If you have some advance notice*, then please let me know as soon as possible, so we can make arrangements for an early exam.
    - *If something happens on the day of the exam that prevents you from taking the exam*,
      - Please send me a message (either Slack DM or email), as soon as reasonably possible.
      - If you have a good reason for missing an exam, I will give you a couple of options on how to “makeup” the missed exam.
    - *Please provide documentation of your absence, if possible.* Examples of such documentation in the past have included flight/travel itinerary or a doctor's note. Particularly with any illness or emergency related to COVID-19, documentation might not be feasible. As a result, I will need to count on each of you to conduct yourselves honorably in this class, particularly as it relates to our exams.
  13. **What happens if there is an emergency on exam day that impacts the entire class?** I will use Slack and Lulima to provide updates.
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### PROBLEM SETS (HOMEWORK)

1. **Successful completion of the problem sets and thorough review of the problems with the posted answer key are essential for building a strong skill set and a reasonable working knowledge of quantum chemistry and spectroscopy.** As such, few students earn a good (or even passing) grade in CHEM 352 without doing the problems.
2. **Your Problem Sets will be posted and submitted via Lulima.** Due dates will be announced in class. You should expect a problem set every 1-2 weeks.
3. **Late homework is accepted for most assignments.** Late assignments will have a penalty of 20% per day. Note that only 1-2 additional (calendar) days are typically given for late homework.
4. **Solutions to the homework will be posted shortly after the deadline at our Lulima site.** For obvious reasons, problem sets will not be accepted after the solutions are posted.
5. **The “homework grade” is the average of the PS scores.** You should expect 8-10 problem sets over the semester.

## GENERAL CLASS POLICIES

These class policies are intended to create, build, and sustain an environment that is conducive to learning (and teaching!) and supportive of our individual and collective goals. Modifications have been made to my class policies, as CHEM 352 in Spring 2021 must be conducted “100% online”. Because constantly evolving conditions of the pandemic may result in additional changes, your cooperation and understanding is and will be greatly appreciated.

**1. Success usually comes with regular attendance and timely completion of reading and problem assignments.** I suggest the following strategies for your success:

- **Prepare for my lectures and attend class consistently.**
  - **Read the book.** This syllabus gives the sections of the textbook that align with my lectures. I will also refer to the book in class on a regular and consistent basis.
  - **Download handout(s) before class.** Find handouts on Lulima (under “Resources”).
- **Take good notes by hand. Review your lecture notes shortly after class is finished.**
- **Use the recorded lectures to fill in gaps, review the day’s material, etc.** I will record all of my classes and will upload them to our Lulima site. The PowerPoint files that I use for my lectures will be viewable on the recorded lectures, but they will not be posted or shared. The recordings should always be considered as a “fall-back” (for your own notes) and not a replacement for coming to class.
- **Do the homework problems in a timely fashion.**
- **Do not wait until the last minute/hour (or day!) to study for an exam.** In normal times, I would include this statement: *“On the day of and the day before an exam, I do not answer questions about the exam material. You must manage your time effectively and be responsible for the outcome of these exams and this class.”* During this unusual time, however, I am relaxing this rule to a limited extent. Please be thoughtful and reasonable, if you are sending a last-minute question – and be realistic about the possibility that I may not respond before the exam.

**2. Seek help when you have questions.** The most efficient way to communicate with me is *(usually!)* face-to-face. However, in the Spring 2021 semester, I welcome your questions and discussion via Slack and Zoom.

- My CHEM 352 “office hours” will be held via Zoom, when needed. (Dates/times TBA)
- If you would like to set up an appointment, please send a message (preferably DM on Slack), with two or more times that you are available.
- Please try to prepare for your meeting with me, as best as you can. If possible, have detailed questions about, e.g., a specific homework problem (or a specific type of homework problem).

**3. Any student who feels she/he/they may need an accommodation based on the impact of a disability should contact the KOKUA Program** (Office for Students with Disabilities) to ensure reasonable accommodations in CHEM 171. KOKUA can be reached at (808) 956-7511 or (808) 956-7612 (voice/text) in room 013 of the Queen Lili’uokalani Center for Student Services.



4. **My lectures and associated (original) course materials (handouts, exams, quizzes, PowerPoints, etc.) belong to me. They are considered my intellectual property.** Some materials are copyrighted by the publisher of our textbook.
  - You are allowed to view the recorded lectures during the Spring 2021 semester. I prefer that you use the uploaded lectures on Lulima, as opposed to recording them on your own.
  - You are not permitted to share the recorded lectures (regardless of source) -- or any original course materials -- with anyone who is not registered in this class at any time (now or future).
  - In addition, posting a Zoom recording to any site (other than Lulima) carries the “potential risk of exposure and violation of FERPA consent requirements, depending on the recording’s contents”.
  - The lectures and any course material may not be posted to any public or private website. You are not allowed to sell or share exam or quiz questions.
  
5. **Let’s work together to create an optimal learning and working environment.** Even in the midst of these most unusual times, there are ways to make this experience effective and (hopefully!) enjoyable. However, I need your collective and individual help.
  - **Let’s begin our class on time.** Please be ready to start at 9 a.m. HST
  - **Please be courteous, if you are late.** Better to come to class a little late than not at all! However, if you think you might be regularly late, please let me know, as a courtesy.
  - **Plan to stay until the end of the class period.** Please let me know, if you will need to leave early on a regular basis, again, as a courtesy. On occasion, I may run slightly overtime, so I ask for your understanding and cooperation in advance.
  - **Minimize distractions to yourself and others.** Try to find the best place to setup, so you can “attend class” in a quiet place with few distractions. Put your phone into ‘do not disturb’ mode, so you are not distracted by texts, phone calls, or social media.
  - **I will typically mute all of you to optimize the quality of the stream (Zoom).** I may also ask that we stop our video for the same reason. However (!), please ask questions, as they arise – and I hope that you will fully engage with me and the rest of the class, when it’s appropriate (e.g., Zoom breakout rooms).
  
6. **Monitor your hawaii.edu email address and our Slack channels for announcements and other class information.** As previous semesters have shown, it may be necessary for me to send information to you, outside of our designated class meeting time on Tuesday and Thursday mornings. If you do not monitor your email address, it is possible that you will miss this information from me. *(If you do not monitor your hawaii.edu address, you bear the responsibility for missing any information that is sent to it.)*
  
7. **Any changes to the class structure or schedule will be announced and/or confirmed via email.** I will also announce these changes in class. Major changes to the class will be confirmed with a revised syllabus. Note that these “major changes” typically result from an unusual and severe emergency, such inclement weather or, as we have seen, a global pandemic.
  
8. **Please let me know if you have any questions about my course. I look forward to working with you!**