Chemistry 432 - Physical Chemistry II
Course Syllabus
Fall 2022

1. Instructor: Dr. David L. Freeman
   Phone: 874-5093
   Office: Beaupre 474 C
   e-mail:dfreeman@uri.edu
   Office Hours: MWF 11. Office hours can either be in person or virtual. For virtual office hours, arrangements must be made in advance with the course instructor. The web address for virtual office hours is https://rhody.webex.com/meet/dfreemanuri.edu. If you are unable to make normal office hours, please let me know in person or by email so that we can make an appointment.

2. Scheduling: MWF 10, Beaupre 105 A

3. Emergency Scheduling: While we expect to have in-person lectures for the entire semester, nobody can predict the actual course of the Covid pandemic. We need to be prepared for one contingency where I (the instructor) test positive for Covid and cannot come to campus. If I catch Covid, and I am physically able to teach from home, we will have virtual, online instruction. If ill, I will present online lectures at the usual class time using the web link
   https://rhody.webex.com/meet/dfreemanuri.edu. In such a circumstance, I will send email to the class providing details about such online lectures.

4. Mask Requirement: The University is committed to delivering its educational mission while protecting the health and safety of our community. While the university has worked 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. Visit web.uri.edu/coronavirus/ for the latest information about the URI COVID-19 response.

   · Universal indoor masking is required by all community members, on all campuses, regardless of vaccination status. **In CHM 432, masks are required for the entire semester**.

· Students who are experiencing symptoms of illness should not come to class. Please stay in your home/room and notify URI Health Services via phone at 401-874-2246.
· If you are already on campus and start to feel ill, go home/back to your room and self-isolate. Notify URI Health Services via phone immediately at 401-874-2246.

If you are unable to attend class, please notify me prior to the start of class at 874-5093 or dfreeman@uri.edu.

5. Text:
   (a) Thomas Engel, "Quantum Chemistry and Spectroscopy," Pearson, Benjamin Cummings, 2019, Fourth Edition
   (b) Thomas Engel and Philip Reid, "Thermodynamics, Statistical Thermodynamics and Kinetics," Pearson, Benjamin Cummings, 2019, Fourth Edition
6. Prerequisites: CHM 192 or CHM 112, MTH 142, PHY 112 or 204, CHM 431. Knowledge of the material in these courses will be assumed.
7. WWW course home page: http://www.chm.uri.edu/courses/?chm432&1
8. Course requirements:
   (a) Hour Exams (Friday, February 18; Friday, March 11; Friday, April 1; Friday, April 22- All exam dates subject to change.) 400
   (b) Final exam (Friday, May 6, 11:30 AM - 1:30 PM) 200
   (c) Total 600

   Grades will be determined on a curve. Incompletes will be given only for documented medical reasons. In the case of an exam missed for a valid medical reason, discuss options with the instructor. If an exam date is canceled owing to weather or any other reason, the exam will be given on the next date the class meets.
9. Anti-Bias Syllabus 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.
10. Disability Services for Students Statement: 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.

11. Academic Enhancement Center: Located in Roosevelt Hall, the AEC offers free face-to-face and web-based services to undergraduate students seeking academic support. Peer tutoring is available for STEM-related courses by appointment online and in-person. The Writing Center offers peer tutoring focused on supporting undergraduate writers at any stage of a writing assignment. The UCS160 course and academic skills consultations offer students strategies and activities aimed at improving their studying and test-taking skills. Complete details about each of these programs, up-to-date schedules, contact information and self-service study resources are all available on the AEC website, uri.edu/aec.

12. Course Goals:

    As can be made clear by examining your textbooks, physical chemistry is subdivided into a number of distinct topics. Last semester you learned the laws of thermodynamics which govern the behavior of chemical systems at equilibrium. This semester we will extend our understanding of the laws of chemistry to the microscopic and non-equilibrium domains.

    One of the major cultural and intellectual achievements of the twentieth century has been the discovery of the laws of quantum mechanics. Although a complete introduction to quantum theory requires one year, we will be able to *understand some of the principles of quantum mechanics and the implications of the theory to chemistry*. This is our first course goal. Closely allied with a discussion of the laws of quantum theory is *to understand elementary atomic and molecular electronic structure*. This second course goal is a consequence of quantum mechanics. Another consequence of quantum theory has been the field of spectroscopy. *Understanding how spectroscopy is used to determine the microscopic properties of molecules* is our third course goal. Although much insight can be obtained from the microscopic laws of nature, it is important to learn the connection between the microscopic laws and the thermodynamics you learned last semester. We meet this goal in an approximate way by studying kinetic theory. Kinetic theory not only gives an ideal-gas molecular description to some of the macroscopic laws of nature, but kinetic theory is also useful in meeting the last goal of CHM 432. Our final course goal is to leave the equilibrium domain *to begin to obtain an understanding of non-equilibrium phenomena*. We shall study non-equilibrium phenomena within the context of the kinetic theory of matter and the study of chemical reaction kinetics. If time permits at the end of the semester, we will also give an introduction to statistical mechanics, which provide a rigorous connection between the microscopic and macroscopic laws of nature.

13. The CHM 432 Web page:

In this course all problem sets, problem set solutions and quiz solutions are to be distributed on the course web page. No paper copies of the problem sets are to be distributed. The URL of our course web page is
http://www.chm.uri.edu/courses/?chm432&1 . It is strongly suggested that you link to our web page to obtain the first problem set as soon as possible.

It is expected that for most of you, success in this course will require some level of help beyond classroom instruction. Because some of you may find it difficult to come to the scheduled office hours, we have installed as part of our course web pages, a page that can be used to submit questions. Questions are submitted by anyone in the class by filling out a form on the web page, and answers are distributed either to the entire class or only to the person asking the question. If the entire class is to receive a copy of the question and answer, the question is treated as anonymous; i.e. the person who asks the question is never identified. In fact, it is possible to submit a question so that even the instructor does not know who submitted the question. Anonymous questions and responses by the instructor are distributed automatically to everyone in the course. With ordinary electronic mail, there is a private correspondence between the student and instructor. By using the web page, the entire class has an opportunity to learn from the questions submitted.

The use of the web page does not preclude personal interaction between any of you and the course instructor. Dr. Freeman has regular office hours, and you are all encouraged to make use of these hours. Alternate meeting times can be arranged by appointment. Additionally, you can contact Dr. Freeman by e-mail or telephone. The e-mail address and phone number for Dr. Freeman is given on the first page of this syllabus.

Any student in CHM 432 can submit questions and comments to Dr. Freeman. Submission of such comments or questions must be made using the WWW home page for this course. The address (URL) of our home page is
http://www.chm.uri.edu/courses/?chm432&1 . To submit a question to the list, you must click on the highlighted text that says "submit a question to the CHM 432 list." As an example of how to use the list, suppose a student in our class, Ms. Benzene Ring, wonders, "What are the units of wavefunctions?" (If you don't know what this means, don't worry. You will understand the question early in the semester). To obtain an answer to her question, Ms. Ring links her web browser (e.g. Firefox or Microsoft Internet Explorer) to http://www.chm.uri.edu/courses/?chm432&1, and she then clicks on the text linking her to the page for questions (i.e. the highlighted text that says "submit a question to the CHM 432 list"). Ms. Ring then enters her e-mail address in the appropriate box and specifies whether she wants her question to be answered to the entire CHM 431 class or to her alone. Ms. Ring then types in the large box

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What are the units of wavefunctions?
```

Ms. Ring then clicks the "send" button. Ms. Ring's question is received by Dr. Freeman. Dr. Freeman then sends an e-mail message to the whole list that might be

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Subject:  wavefunction units
The question is:  What are the units of wavefunctions?
Answer:  In one dimension, the units are 1/\sqrt{length}.
In three dimensions the units are 1/\sqrt{volume}.
```

Now Ms. Ring and the entire class have an answer to her question. In the answer \sqrt{} stands for a square root, and this notation is discussed below.

If the answer to the question can be sent to the entire list, the answer will not indicate who asked the question. If Ms Ring wants to ask the question with full anonymity so that even Dr. Freeman has no idea who asked the question, the e-mail portion of the form can be left blank. Of course, if the e-mail section of the form is blank, the answer must be sent to the list and not just to the sender.

Because many questions may contain mathematical formulas, we need a notation to communicate the special symbols used in the course. To avoid confusion, it is most useful if we agree on the same set of symbols. The symbols that follow are taken from a language called LaTeX. LaTeX is a language that is frequently used to prepare scientific documents, and LaTeX can be used to translate special symbols into simple text characters. By learning LaTeX notation, you will learn a widely used method to communicate mathematical symbols via e-mail. The instructor plans to use these symbols in answering your questions, and it is asked that you use the same symbols in posing questions. The most important symbols are the following:

(a) Greek letters are represented by \ followed by the name of the letter. For example α is typed `\alpha`, β is typed `\beta`, and so on. A Greek letter is made upper case by making the first letter of its name upper case. For example, the letter Δ is typed `\Delta`.

(b) Subscripts are represented by _{} where the brackets contain the subscripts. For example, μ_{ij} is typed `\mu_{ij}`.

(c) Superscripts are represented by ^ {} where the brackets contain the superscripts. For example, β^{12} is typed `\beta^ {12}`.

(d) Infinity (∞), is typed `\infty`.

(e) The integral sign $\int$ is typed `\int`. The limits on a definite integral are included by introducing subscripts and superscripts. As an example $\int_0^\infty e^{-x^2} dx$ is typed `\int_{0}^ {\infty} e^ {-x^ {2}} dx`.

(f) The partial derivative symbol ∂ is typed `\partial`.

(g) The summation sign $\sum$ is typed `\sum`. The lower and upper limits of summation are included as subscripts and superscripts. As an example $\sum_{n=0}^{\infty} 1/n^2$ is typed `\sum_{n=0}^ {\infty} 1/n^ {2}`.

(h) Square roots $\sqrt{a+b}$ are typed `\sqrt{a+b}`.

(i) The arrow in chemical reactions $\rightarrow$ is typed `--->`. For example $C{+}O_2 \rightarrow CO_2$ is typed `C + O_{2} ---> CO_{2}`.

Let us now look at another example of a question submitted using the web. In this case, Ms. Ring has a question requiring an equation. This might be a real question. If you don't understand the context, don't worry. You will understand the details of the question later in the course. Suppose Ms. Ring wants to ask

"In calculating an expectation value, the expression is

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi dx$$

For calculating the expectation value of the momentum, what operator do we use for A?"

To submit the question, Ms. Ring uses her web browser to attach to http://www.chm.uri.edu/courses/?chm432&1, clicks on the line that says, "submit a question to the CHM 432 list," and then Ms. Ring enters the information requested by the form. If Ms. Ring wishes to remain anonymous, Ms. Ring leaves the e-mail box blank. Ms. Ring then types into the large box

```
In calculating an expectation value, the expression is
< A > = \int_{-\infty}^ {\infty} \psi^ * A \ psi dx.
For calculating the expectation value of the momentum, what operator do we
use for A?
```

and clicks on the submit button. Ms. Ring's question is received by Dr. Freeman. The answer will be sent either to Ms. Ring alone, or preferably to the entire class if the appropriate box is checked. Dr. Freeman might reply

```
Subject:  Momentum Operator
The question is:In calculating an expectation value, the expression is
< A > = \int_{-\infty}^ {\infty} \psi^ * A \ psi dx.
For calculating the expectation value of the momentum, what operator do we
use for A?

The answer is:  A=p=hbar/i d/dx
```

14. Course outline[1]:

Topic	Book Chapter
1. Review of Classical Mechanics and the Quantum Nature of Matter	(a) 1, 6.3
2. The Schrödinger Equation	(a) 2.2-2.5
3. The Postulates of Quantum Mechanics	(a) 3
4. Simple Quantum Systems	(a) 4, 5.5
5. Vibrational and Rotational Motion	(a) 7
6. Vibrational and Rotational Spectroscopy of Diatomic Molecules	(a) 8.1, 8.3-8.6, 8.8
7. The Hydrogen Atom	(a) 9
8. Many-electron Atoms	(a) 10.1-10.4
9. Atomic Spectroscopy	(a) 11.1-11.4
10. Chemical Bonding	(a) 12, 13.8
11. Molecular Electronic Spectroscopy	(a) 14.1-14.4, 14.6-14.8
12. Kinetic Theory	(b) 16, 17
13. Chemical Kinetics	(b) 18
14. Statistical Mechanics (time permitting)	Handout
15. Final Exam	Comprehensive

[1](a) = "Quantum Chemistry and Spectrocscopy," (b) = "Thermodynamics, Statistical Thermodynamics and Kinetics"