Syllabus
Physical Chemistry II (CHM 3411)
Spring 2018

Basic Information

Instructor: David Chatfield, CP 336, 305-348-3977, Chatfield@fiu.edu, https://casfaculty.fiu.edu/David.Chatfield/

Course Description in a Nutshell: The course introduces quantum mechanics as applied to chemistry. After a careful introduction to the principles, we will build to the subjects of atomic and molecular orbitals, chemical bonding, spectroscopy, and computational chemistry.

Prerequisites: CHM 3410. Note that the prerequisites for CHM 3410 include two semesters of calculus and two semesters of physics with calculus, so you should have all of that under your belt.

Class Time and Place: MWF 12:00-1:15 P.M., SASC 352

Canvas (at online.fiu.edu): Most course materials, including problem sets, problem set solutions, reading assignments, and exam grades, will be made available on Canvas. You should check Canvas before every class, particularly because reading assignments will be adjusted depending on the progress made in the previous class. To login to Canvas, go to online.fiu.edu and use the username and password you use for most FIU online tasks. Once logged in, look for this class.

Office Hours: Chosen: M 4-5 pm, T 11-12 noon. (DONE: During the first two weeks of class we will choose a time that works well for both students and the instructor.) No choice will work for everyone, so you are welcome to come by my office at other times. I will work with you then if I can, and if I can't (like everyone, I have many responsibilities), I will be happy to arrange a time in the near future. You can also email me to arrange a time.

Exams dates (see description of grading below):

Midterm Exams 1 and 2: The ***tentative*** dates are Feb 12 and Mar 9, respectively. However, I will survey you during the second week of class to find out when exams are scheduled in your other classes and avoid them if possible. No dates will be perfect for everyone, but we will try to find the dates that are best for the most students. ***Our firm exam dates will be announced by the beginning of the third week of class***.

Midterm Exam 3: (Wed Apr 20 firm)

Final Exam: (TBA, will be set by University and be firm)

Make-up Exams: Students are expected to take exams on the regular exam dates. Make-up exams are offered only in extraordinary circumstances and only if advance arrangements are made.

Texts: Required: Peter Atkins and Julio de Paula, *Physical Chemistry, 10th Ed.*, Freeman, 2014, ISBN-13: 978-1429290197.

You probably already have this text, as it was used in Physical Chemistry I in Fall 2017. If not, it is available at FIU's Barnes & Noble Bookstore and online (e.g. amazon.com); as hardback or digital; for purchase or rent. If you own an earlier edition, it is probably sufficient for learning, but you are responsible for any new material in the current edition and for any changes in the problems assigned at the end of the chapter.

Recommended: James R. Barrante, *Applied Mathematics for Physical Chemistry, 3rd Ed.*, Waveland Press, 2016, ISBN-13: 978-1478632474 (formerly published by Pearson Education).

This is a great little volume that reviews mathematical techniques used in physical chemistry. It also provides practice problems for honing your skills. It is not a required text, but I strongly encourage you to get this book. We will use a number of mathematical approaches you have not used before in the chemistry curriculum. They are introduced in Atkins, but the coverage in Barrante is excellent and very helpful. Barrante will be a valuable reference for you later, too.

Computational Chemistry: Computer software allows us to calculate many properties of molecules and to visualize the results in helpful ways. We will introduce the program Spartan early in the course, and you will use it in lab as well as lecture. You will be able to access the program using your personal laptop. *If you do not own a personal laptop, please let the instructor know right away so that we can find an alternative for you.*

Computational problems will be assigned periodically throughout the semester. These will reinforce points learned in class and principles encountered elsewhere in the chemistry curriculum. They will also equip you to use computational chemistry techniques after this course. The use of computational chemistry in combination with experiment is growing rapidly, so this will be a useful skill for you.

All computational methods are approximate to some degree, and choosing the appropriate method for a given problem is a skill that must be learned. At the beginning of the course, you will always be instructed what method available in Spartan is appropriate for each problem. Later in the course, you will learn the theory behind some of the methods and how to make appropriate choices.

Why should you care about quantum mechanics?

Describing nature at the sub-microscopic scale requires different models (of stuff and the way stuff interacts with other stuff) from those that work successfully at the larger scale. Because chemistry depends on very small things (basically, how electrons and nuclei interact with each other and with light), you need to understand these models if you want to develop a deep understanding of chemistry. The term for these models – the physical laws and the concepts – is quantum mechanics.

Quantum mechanics will help you understand all of chemistry more deeply because you understand the fundamentals more deeply. That in turn will help you design experiments, formulate synthetic routes to create new molecules, understand spectra, predict how biomolecules will interact, and on and on. When you have a deep understanding of the fundamentals, you will be set to expand your knowledge in many creative directions.

If quantum mechanics is so fundamental, why are we only learning about it now?

Actually, you have already learned some things about quantum mechanics in general chemistry and later courses. For example, atomic orbitals (s, p, d, f), the energy levels of atoms, the periodicity of the periodic table, and molecular orbital theory are all concepts from quantum mechanics. However, the mathematics of quantum mechanics is more sophisticated than that needed earlier in the chemistry curriculum. You need two semesters of calculus and two semesters of physics before trying to understand the theory behind quantum mechanics in depth, so quantum mechanics is usually a junior- or senior-level course.

Does this mean everything you have learned earlier in chemistry was premature? No, of course not! Learning is a layering process. You don't learn everything there is to know about organic chemistry, and then turn to analytical chemistry, and so on. Rather, you learn the basics of each subject, and then return to each subject and deepen your knowledge, over and over (your whole life long!). Once you have learned about quantum mechanics, you will be ready to understand other subjects in chemistry more deeply.

How will you succeed in the course?

Study regularly. Cramming for exams will work even less well in this course than in most others because the learning is scaffolded. Each topic we cover builds on the previous topics. If you miss early material, it will be very hard to learn later material.

Furthermore, the exams require analysis and creative thought, not just recall. Quantum mechanics is not about memorizing equations and terms. Over the years, students have remarked to me time and time again that they stayed up late cramming, only to find in the exam that they just couldn't think well enough to approach the questions. To succeed in the course, you need to spread your studying out over time.

Read the text early. Skim a new chapter first to figure out where it is going. Then read each section before we cover it in class. This will set you up to understand class better and ask questions where you have difficulty. Later, read the section more thoroughly. You should find that the in-class work and the text are complementary, each providing insight into the other.

Work lots of problems, and with a strategy. Problem solving is the heart of learning physical chemistry. When you solve problems, you are putting the concepts and mathematical machinery to work. Your brain will be forging new connections. Use a good strategy. Begin each chapter's work with easy problems. They are the first ones at the back of the text. They generally apply concepts and equations in a straightforward manner. I call these warm-ups. You do warm-ups in sports, right? Stretch, dribble the basketball, take some practice tennis serves, swim a couple laps at half speed. Why not do the same when studying? Some of the warm-up problems may seem overly simple: do some anyway! They will bring the concepts and equations to the front of your mind, preparing you to tackle the more advanced questions.

The more advanced questions will combine several concepts and equations from the chapter, and perhaps draw on other chapters and prior coursework. They should challenge you. If you find yourself continuously struggling, though, you might try going back and doing more warm-ups and then returning to the challenging problems. If you feel under-challenged, try more difficult problems (feel free to see me for suggestions).

Milk the problems. You will spend a lot of work on some problems. Don't let that work go to waste. Build on it! Turn your answer over in your mind. Ask yourself whether it is physically plausible. Think about the different concepts it combines. Ask yourself what other chemical concepts it is related to. Remind yourself what made your approach work for this problem, so you know to approach other related problems in a similar way. This way you will be deepening and broadening your learning. If you take 5 minutes to do this after spending 15 minutes solving a problem, you will double or triple what you get out of it. That's a good pay-off!

Get help soon if you are having trouble. I'm here to help you. Ask me a question after class, come to office hours, email me for a time to meet, or simply email me a question. Other students are also a great resource. Don't wait to see whether something will make better sense if you give it a week or two. This course builds rapidly, so clear up confusion right away. Otherwise it will be hard to learn the next material.

Study groups. Many minds are often better than one. You can learn a lot from your peers. Working in teams is expected in today's job market. But be careful: **the one who does the work does the learning**. When you are working in a group, you need to be actively involved for your time to be well spent.

Have a strategy for studying for the exams. Don't cram. The exam date will be announced well in advance. Reviewing the text and class notes, reviewing problems, and working more problems will prepare you for the exams. Give yourself plenty of time to do all these things. I recommend that you begin reviewing the exam material at least a week in advance and plan how you will allot your time. Get plenty of sleep the night before the exam because you will need to be able to think creatively in the exam. My exams are not memory dumps.

How is the course organized?

There are basically five sections to the course:

Failures of classical physics (the prelude). These are the experiments of the late 19th and early 20th centuries that revealed the inadequacy of the laws of physics, as then understood, to describe matter and energy at the sub-microscopic scale. This led to the discovery of the laws of quantum mechanics.

Principles of quantum mechanics (the foundation). We will learn about the principles of quantum mechanics, preparing the introduction of the Schrödinger equation. Together, the principles and the Schrödinger equation are the foundation for the rest of the course. We will also take time to explore mathematical techniques and principles that may be new.

Model problems (the warm-up). We will apply the Schrödinger equation to several model problems (particle-in-a-box, tunneling, rigid rotor, harmonic oscillator). The model problems were selected to represent key features of atoms and molecules (although this may not be immediately apparent). Tackling the model problems in isolation helps us understand these key features deeply. Later, when we study real molecules using quantum mechanics, we will build upon the concepts and mathematical solutions developed with the simple models. Be patient with these model problems, even if their relevance for chemistry is not immediately apparent. Rome was not built in a day!

Chemical applications of quantum mechanics I: Atomic and Molecular Structure (the first pay-off). Here is where our earlier work will begin to pay off. We will apply quantum mechanics to understand a host of phenomena and concepts central to chemistry: the electronic structure of atomics and molecules, chemical bonding, valence bond theory, molecular orbital theory, and more.

Chemical applications of quantum mechanics II: Spectroscopy (the second pay-off). Our earlier work will continue to pay off as we learn how the interaction of light with molecules reveals much about molecules' properties and structure. We will explore several kinds of spectroscopy, including microwave, infrared, ultraviolet-visible, Raman, NMR, and EPR. The framework of quantum mechanics will deepen your understanding of these topics, some of which you will have encountered earlier. We will also take a brief look at the principles of lasers.

Learning Outcomes (What will you learn?)

Course specific outcomes

- Develop an understanding for how nature works at the atomic and molecular scale, based on the principles of quantum mechanics.
- Solve the Schrödinger equation, using appropriate boundary conditions, to determine the accessible states of simple physical systems.
- Use and understand the language of quantum mechanics – the terms and concepts – to describe chemical phenomena.
- Based on insights from quantum mechanics, deepen your understanding of:
    - Chemical bonding (what determines the energies, strengths and orientations of covalent bonds)
    - Molecular structure (why molecules have the structures they do)
    - Chemical reactivity (how and why chemical reactions take place)
    - The principles of spectroscopy (microwave, UV-Vis, NMR), that is, of what we can learn about molecules from their interaction with light
- Use computational chemistry software to predict properties of molecules.

Over-arching outcomes

- Hone your problem solving skills:
    - Formulate an approach to a problem.
    - Apply conceptual and mathematical relationships to solve a problem.
    - Assess whether a solution is physically plausible.
    - Interpret quantitative solutions conceptually.

- Use approximations wisely: recognize when approximations are made, determine whether approximations are adequate and how to go beyond them, and use approximations to develop understanding (back-of-the-envelope calculations).
- Use visual techniques (figures and graphs) to illustrate physical and mathematical relationships and develop conceptual understanding.
- Describe chemical concepts in your own words and in technical language, understanding the advantages of each kind of description (situation/audience appropriateness).

How will you be evaluated (the nitty and gritty of grading)?

Grades will be based on three Midterm Exams (55%), a Final Exam (35%), and Homework (10%). I use a modified absolute scale for assigning grades. Over the years, I have developed an ***approximate*** numerical grading scale that represents your learning. That ***approximate*** scale is A:75-100, B:65-74, C:55-64, D:30-54, F:0-29 (with + or – at the ends of the ranges). Why do I say approximate? Exams vary slightly in difficulty from year to year. I write them fresh, and that's just the way it turns out. Therefore, I may curve each exam slightly in view of the difficulty (by curving I mean assigning a letter grade to a numerical score range). You will know where you stand from your letter grade on each exam. The overall scale at the end of the course will reflect the curving of all the exams. The important point to remember is that the grades are designed to reflect your absolute learning, not just your learning relative your peers in this class. If everyone does great, everyone will get an A. It hasn't happened yet, but it could.

Midterm Exams: These are to give you and me feedback on your progress and to incentivize you to keep learning steadily. The Midterms will focus on new material, but the most important points from earlier material are also fair game. This means that you should always be alert to sift and evaluate what the most important ideas are as we go along. I will give guidance, but you as a learner must take ownership for evaluating what ideas/concepts/skills are truly key. The last Midterm will be on the next to last day of class. This will encourage you to review the last material covered in depth and allow the Final to be truly comprehensive. I also have a policy of allowing you to recover from a poor performance on one Midterm: if your performance on the Final is better than on your lowest-scoring Midterm, I will replace a portion of that lowest-scoring Midterm grade with your score on the Final (more precisely, your new Midterm score will be 80% of your score on the Final plus 20% of your original score on the Midterm, with all scores first converted to a 100-point basis).

Final Exam: The Final will be comprehensive. Its purpose is to give you and me feedback on your overall learning in the course, and to incentivize you to undertake a serious, in-depth, comprehensive review as the final component of your course learning.

Homework: Problem sets will be assigned by Monday of most weeks and will generally be due in class the following Monday; this pattern may be altered for exam weeks or holidays. Late homework will not be accepted. Problem sets and their solutions will be posted on Canvas. Problem sets will be graded on a check or check-minus basis set, with check-minus receiving half credit. Solving problems involves multiple skills and is the way best way to deepen your learning. I strongly suggest you do warm-ups (simple problems) before proceeding to the more challenging problems (see Learning Outcomes section). **Be sure to keep up with the homework. Regular practice with the material as you progress through the course is very important for your learning.**

Course Schedule (may vary depending on class progress)

Week	Chapter	Topic
1	7	Failures of Classical Physics
1	Suppl*	Introduction to Computational Chemistry Software
2	7	Quantum theory: introduction and principles
3	8	Quantum theory: techniques and applications
5	9	Atomic structure and atomic spectra
7	10	Molecular structure
8	10+Suppl*	Computational Chemistry
9	11	Molecular symmetry
10	12	Molecular spectroscopy 1: rotational and vibrational spectra
12	13	Molecular spectroscopy 2: electronic transitions
13	14	Molecular spectroscopy 3: magnetic resonance

*Supplementary material to be made available

Your ethical responsibility

Florida International University is a community dedicated to generating and imparting knowledge through excellent teaching and research, the rigorous and respectful exchange of ideas, and community service. All students should respect the right of others to have an equitable opportunity to learn and honestly demonstrate the quality of their learning. Therefore, all students are expected to adhere to a standard of academic conduct, which demonstrates respect for themselves, their fellow students, and the educational mission of the University. All students are deemed by the University to understand that if they are found responsible for academic misconduct, they will be subject to the Academic Misconduct procedures and sanctions, as outlined in the Student Handbook.