Chem 3420 – Quantum Theory

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Course Description and Goals

Physical Chemistry describes and develops the foundations of the broad subject of chemistry in terms of fundamental concepts of physics, using the language of mathematics. As such, it represents a very broad subject matter and all of chemistry is built on this foundation. We focus on the two fundamental aspects: quantum mechanics, which focuses on the energy states of individual atoms and molecules; and thermodynamics, which covers the transformation of energy in the form of heat and work within bulk ensembles of matter. A third area covers the intersection between these two disciplines: statistical mechanics, where the tools of statistics are used to develop thermodynamic quantities from the energy levels of individual atoms and molecules.

The subject that we will cover this semester is quantum mechanics with specific application to atomic and molecular systems. We will cover topics ranging from the electronic structure of individual atoms to the nature of the chemical bond in polyatomic molecules. We will end with an introduction of statistical mechanics which will provide a basis for topics covered in the next semester.

The broader goal of this course is to provide you with the skill to use the language of mathematics to describe natural phenomena, as well as the ability to apply this skill in a variety of different contexts. This will enable you to effectively engage with the scientific community and absorb quantitative aspects of the scientific literature.

Class: MWF 10:00 – 10:50 AM Ruffner Hall G006.

Review sessions: Friday 2:00 − 3:30 PM Ruffner Hall G006.
These optional sessions are conducted by our TA, Sean Schulte, and will be used to cover mathematical background (Math Chapters), homework, and general discussion about the material covered in class.

Main text: Physical Chemistry, A Molecular Approach
by Donald A. McQuarrie and John D. Simon; University Science Books.
There is a companion solutions manual (recommended) with worked out solutions to textbook problems.

Optional text: Physical Chemistry (Third Edition)
by Thomas Engel and Philip Reid; Pearson.
This book can be useful to get a second perspective on the subject.

Office hours:	Sean Schulte	Wednesday, 1:00-2:00 PM	Chemistry 150
	Andreas Gahlmann	Tuesday, 5:00-6:00 PM	Chemistry 124

Approximate Course Schedule

Week			Chapter	Section	Topics
1	Aug	25*	Chapter 1 Chapter 2	1.1−1.8	Failures of Classical Mechanics, Dawn of Quantum Mechanic (Chapter 2 covered in Review session)
2	Sept	1	Chapter 3	3.1−3.9	Operators, The Schrödinger Equation, Interpretation of the Wave Function; Particle in a box
3		8†	Chapter 4	4.1−4.6	Tunneling, Postulates of Quantum Mechanics
4		15	Chapter 5	5.1–5.9	Spectroscopic Models: Harmonic Oscillator, Rigid Rotor
5		22†	Chapter 6	6.1–6.7	The Hydrogen Atom; Atomic Orbitals
6	**Sept**	**29**	**Exam I: Chapters 1 through 4 (Time TBA for Exam)**		
6		29	Chapter 6	6.1–6.7	The Hydrogen Atom; Atomic Orbitals
7	Oct	6†	Chapter 7	7.1–7.4	The Variational Method
8		13*	Chapter 8	8.1–8.11	Multielectron Atoms; Electron Spin Antisymmetric Wavefunctions; Slater Determinants; Term Symbols
9		20†	Chapter 9	9.1–9.9	The Chemical Bond; Molecular Orbitals
10		27	Chapter 9	9.10–9.16	LCAO-MOs; Electronic States for Molecules; Term Symbols
11	Nov	3†	Chapter 10	10.1–10.6	Polyatomic Molecules; Hybrid Orbitals; Hückel Approximation for Conjugated Hydrocarbons
12	**Nov**	**10**	**Exam II: Chapters 5 through 10 (Time TBA for Exam)**		
12		10	Chapter 13	13.1–13.7	Molecular Spectroscopy; Rotational, Vibrational, and Electronic Spectroscopy
13		17†	Chapter 13	13.8–17.14	Molecular Spectroscopy; Rotational, Vibrational, and Electronic Spectroscopy
14		24*	Chapter 17	17.1–17.8	Statistical Mechanics: the Boltzmann Distribution and Partition Functions
15	Dec	1†	Chapter 18	18.1−18.5	Partition Functions for Ideal Gases
	Dec	**15**	**Final Exam: (Time TBA for Exam); Comprehensive with emphasis on Chapters 13, 17, and 18.**		

* Classes start Tuesday, Aug. 26th; Fall reading days: Monday and Tuesday Oct 13th and 14th; Thanksgiving recess: Wednesday through Friday, Nov. 26th – 28th; classes end Friday Dec. 5th.

† Problem sets will be due on the Friday of these weeks. All sets due outside my office (Chemistry 129) by 5:00 p.m.

Lecture:
The preceding table is an approximate schedule of material that I will cover during lecture this semester. In general, we will attempt to stay as synchronized as possible with the other section of this class. I will assume that you are comfortable with material covered in the General Chemistry, General Physics, and, most importantly, your Calculus courses. In the lecture, I will give detailed discussions of the specific mathematical operations necessary for solving the problems in quantum mechanics. It will be to your benefit to read the material to be covered in lecture in advance. You will find that, if you try some of the example problems before lecture, your ability to understand the material and follow and engage in discussion will increase dramatically!

Homework:
Problem sets will be provided to guide your study of physical chemistry. I encourage you to use scratch paper to think freely about homework problems after which you should write down the final solution neatly and clearly on white copy paper (stapled together before submission). I further encourage you to work in study groups to work on homework problems. The group will benefit from your participation the most, if you have previously tried to solve the problem on your own and can share your thought processes. Each student must hand in his or her own copy of the homework (photocopies are not acceptable). You may also include printouts from programs like Mathematica, if you are using it to solve homework problems, provided that it is sufficiently annotated, so we can follow your reasoning.
Problem sets will be assigned for collection roughly every two weeks.

Missed Exams:
There will be three exams during the course: two exams during the weeks of Sept. 29th and Nov 10th and the final exam on Dec. 15th. We will attempt to find a time outside of class for the first two exams; these may be during the problem/review sessions in those weeks or in the form of take home exams.
For in-class exams: If you have an unavoidable conflict that precludes you from taking an exam during the specified period, you must contact me prior to the exam as soon as you know that you will not be able to be present during the exam period. Make-up exams will be given at my discretion provided I have sufficient documentation to justify your absence. You must take the final exam in order to receive a passing grade in this course.

Grading:

Exams:	$2 \times 20\% = 40\%$
Final Exam:	30%
Problem sets:	30%
Total:	100%