# *CHEM 1410: Physical Chemistry 1 – Quantum Mechanics*

Fall 2017 · Term 2181
Lecture: TH 1:00 – 2:15 pm · Chevron 150 Ashe Auditorium
Recitation W 2:00 – 2:50 pm · Chevron 150 Ashe Auditorium
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Office hours: T 11-11:50 or by appointment

Last updated 29 August 2017.

## *Goals of the course*

This course, CHEM 1410 Physical Chemistry 1, "Quantum mechanics", builds a conceptual framework to quantitatively and qualitatively analyze the properties of individual atoms and molecules. Physical Chemistry 2, "Statistical mechanics and thermodynamics", builds on quantum mechanics to analyze macroscopic quantities of atoms and molecules, when there are moles of particles. Together, they form a quantitative theoretical foundation for all of chemistry.

**Quantum mechanics** is the set of tools to calculate and interpret systems when they are *small*. Classical mechanics is set of tools to analyze the macroscopic world. The rules of classical mechanics, however, break at a certain length scale, which is around one nanometer. Because atoms and molecules are smaller than this length scale, we need to develop new physical laws to describe this regime. These new physical laws also require us to revise our physical intuitions. Ultimately, all of the richness of chemistry is an expression of the quantum mechanical universe. Why does the periodic table have its structure? What is an orbital? What is the nature of the chemical bond? As chemists, we care deeply about these questions. Quantum mechanics provides the answers.

Our task is to develop tools to answer these questions.

## *Structure of class and assignments*

We will devote our class time to an active investigation and derivation of the *key* concepts that underlie the physics and chemistry.

Most of the assignments for the course will be classic "homework". The homework assignments will be distributed at least a week before they are due. The purpose of these assignments is to give you practice applying the quantitative techniques to simple problems to build your "chemical intuition" and prepare you for the types of questions which will be on the midterms and final exam. Teamwork is great. Science rarely happens alone these days. Solving the assignments will be much more productive if you work together.

*Overarching goals of the class are to improve your ability*

- to build simple models of quantum systems,
- to *quantitatively analyze* the models ("do math"),
- to *interpret* your results ("figure out what it means"),
- to *communicate* your results,
- to work in teams.

*Please note, the exercises will be graded on a 0 – 1 – 2 basis:*

**0** The exercises show no significant progress towards solving the problems.

**1** The exercises show some progress towards solving the problems. The solutions were either not complete or contained major mistakes.

**2** The exercises show substantial progress towards the correct solutions, though there may be errors in detail.

EXAMS will contribute the bulk of your grade. I anticipate 2 take-home midterms and a comprehensive take-home final exam. Exams are individual efforts.

### *Grading*

The points in the course will be broken down as

- Exercises ( 25 % )
- Two midterms ( 50 % )
- Final exam ( 25 % )

### *Required texts*

- Engel "Quantum Chemistry and Spectroscopy", 3rd edition (Pearson).
- Shepherd and Grushow "Quantum Chemistry and Spectroscopy", 1st edition (Wiley).

### *Optional texts (on reserve)*

- D. A. McQuarrie "Mathematics for Physical Chemistry: Opening doors"
- J. R. Barrante "Applied Mathematics for Physical Chemistry"

### *Learning objectives*

In this class you will learn

- To interpret the spectrum of blackbody radiation and the temperature of the emitter
- To analyze the photoelectric effect relating the metal work-function, stopping voltage, the light intensity, and light frequency
- To convert a photon's energy, frequency, and wavelength in various spectroscopic units
- To use an energy level diagram and associated selection rules to predict the energies of absorption or emission of light
- To use a wavefunction to calculate the possible measured values of an operator, both the individual results and the average (expectation value)
- To calculate the commutators of different operators
- To interpret commutators in terms of the uncertainty principle
- To evaluate if functions are eigenfunctions of an operator
- To evaluate the orthogonality of wavefunctions by explicit integration and by symmetry
- To analyze and interpret the eigenenergies and eigenfunctions of simple Hamiltonians (the particle in a box, harmonic oscillator, rigid rotor, and the hydrogen atom)
- To use the language of quantum mechanics to describe systems and measurements precisely
- To analyze and interpret the hydrogen atom wavefunctions, the quantum numbers and the numbers of nodes in the wavefunction
- To use appropriate boundary conditions to select physically acceptable wavefunctions for various problems
- To use the particle-in-a-box model to qualitatively assess a variety of molecular problems

- To assign spectroscopic transitions in different spectroscopies (vibrational, rotational, and electronic)
- To graph wavefunctions in multiple dimensions
- To calculate the probability of finding a particle based on its wavefunction
- To use variational theory for multielectron Hamiltonians (or other complex problems)
- To write electron configurations for ground and excited states of an atom
- To use nuclear charge and shielding to interpret energy trends
- To write correct antisymmetrized wavefunctions for multielectron atoms (Slater determinants)
- To assign term symbols to electron configurations
- To identify correct linear combinations of atomic orbitals for bonding and antibonding molecular orbitals
- To calculate charge density and bond orders from simple molecular wavefunctions
- To identify the electron configuration, bond order, and paramagnetic properties of molecules based on a molecular orbital diagram

*Feedback*

Three times during the semester there will be feedback sessions outside of class for six students to give feedback on how the course is progressing. The sessions are purely voluntary, but participation will be rewarded with 1 homework point. The sign-ups will be first-come first-served through Courseweb.

*Important days*

**Fri 8 Sep: Add/drop deadline**

**Tue 10 Oct: NO CLASS**

**Fri 28 Sep: Midterm 1 take home**

**Fri 3 Nov: Midterm 2 take home**

**Wed 22 Nov – Fri 26 Nov: Thanksgiving NO CLASS**

**Thu 7 Dec: Last class**

**Mon 12 Dec – Fri 16 Dec: Take home final**

*Disability*

If you have a disability for which you are or may be requesting an accommodation, please contact both me and Disability Resources and Services, 140 William Pitt Union, 412-648-7890 as early as possible in the term.

Disability Resources and Services reviews documentation related to a student's disability, provides verification of the disability, and recommends reasonable accommodations for specific courses.

*Integrity*

All students are expected to adhere to the standards of academic honesty. Any student engaged in cheating, plagiarism, or other acts of academic dishonesty would be subject to disciplinary action. Any student suspected of violating this obligation for any reason during the semester will be required to participate in the procedural process, initiated at the instructor level, as outlined in the University School of Arts and Sciences Academic Integrity guidelines at http://www.as.pitt.edu/faculty/policy/integrity.html.

*Classroom recording*

To ensure the free and open discussion of ideas, students may not record classroom lectures, discussion, or activities without the advance written permission of the instructor. Any such recording can be used solely for the student's own private use.

*Religious observances*

Please let me know as early as possible of any conflicts between class activities and religious observances so we can make appropriate arrangements.