

Syllabus CHEM 1410 Physical Chemistry 1 Fall 2018

Lecture: TuTh 1:00 – 2:15 in 150 Chevron
Recitation: We 2:00 – 2:50 in 132 Chevron

Instructor: David Ewing, Ph.D. dwewing@pitt.edu Office: 318 Chevron
Email will normally be answered within 24 hours.

Office hours: Mo 1:00-3:00 in 318 Chevron, We 11:00-1:00 in **501 Chevron**, and by appointment. I will also be available right after most of our classes and recitations.

Course description: This course will introduce quantum theory, atomic and molecular structure, symmetry, and spectroscopy. Detailed topic list: Pre-Quantum Mechanics; Schrödinger Equation; Quantum Mechanical Postulates; Free Particle; Particle in a Box; Tunneling; Operators; Uncertainty Principle; Harmonic Oscillator; Vibrational Spectroscopy; Rigid Rotor; Rotational spectroscopy; Hydrogen Atom; Many Electron Atoms; Diatomic Molecules; Linear Variation Functions; Electron Spin; Hartree-Fock (HF) Theory; Polyatomic Molecules; Hückel Molecular Orbital Theory; Post-HF Methods; Molecular Symmetry; Atomic Spectroscopy; Electronic Spectroscopy

Text: Engle, T. *Quantum Chemistry & Spectroscopy*, 3rd ed.; Pearson, 2013.

We will cover most of the textbook, except the last chapter. Some supplemental topics, or enhancements of topics in the textbook, will occasionally be presented. Some sections of some chapters will not be covered and those will be announced in advance. A class schedule will be maintained as we go along, and posted in the Syllabus section of CourseWeb.

CourseWeb: Course information will be posted at <https://courseweb.pitt.edu>. This will include announcements, lecture notes, homework assignments, your scores, and this syllabus - updated as needed.

How the class will be conducted: Lecture periods will be mostly lecture, with some time devoted to problem solving. Recitation periods will involve problem solving, examlets (see below) and sometimes catching up on lecture material.

Exams & Examlets: The final exam will be comprehensive, and is scheduled for Thursday, December 13, 10:00-11:50 am. There will be a take-home exam about 2/3 of the way through the course. I am open to negotiating the timing of the take-home exam, to fit it in around your other exams. About every other week we will have an "examlet", i.e. extensive quiz. This will help you keep up with the material on a regular basis. The first examlet will be on September 12. There are no make up exams or examlets, and they can be taken early only for valid reasons. Exams and examlets will focus on problem solving.

Homework: Problems will be assigned for each chapter. These will not be collected or graded. I will give you the worked out solutions after you've had time to work on a given assignment. The homework will serve as a basis for the exams and examlets.

Projects: Several small computational projects will be assigned, to be done using software available in the Department. This will give you some practical experience in computational chemistry to go along with the theory we're discussing in class.

Grades:

Examlets	40%
Take-home Exam	20%
Final Exam	20%
Projects	20%

It is anticipated that A/B/C = 90%/80%/70% with pluses and minuses will be used for the course grade, but this could be more munificent at the discretion of the instructor.

Changes to course structure: The Instructor reserves the right to change this syllabus as needed, and will inform the class verbally and on CourseWeb of any changes.

Academic Integrity Statement: Cheating/plagiarism will not be tolerated. Students suspected of violating the University of Pittsburgh Policy on Academic Integrity will be required to participate in the outlined procedure. A minimum sanction of a zero score for the quiz or exam will be imposed. See www.cfo.pitt.edu/policies/policy/02/02-03-02.html.

Disability Resources: If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact both the instructor and the Office of Disability Resources and Services as early in the semester as possible, 140 William Pitt Union at 412-648-7890 or <http://www.studentaffairs.pitt.edu/drs/>

To ensure the free and open discussion of ideas, students may not record classroom lectures, discussion and/or activities without the advance written permission of the instructor. Any such recording, properly approved in advance, is limited to the student's own private use.

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