

Syllabus CHEM 1480 Intermediate Physical Chemistry Fall 2019

MoWe 4:00 – 5:15 in 154 Chevron Science Center

Instructor: David Ewing, Ph.D. dwewing@pitt.edu Office: 1206 Chevron
Office hours: Tu 1:00-3:00 and We 10:00-noon, and by appointment. I will also be available right after most of our classes.

Course description: This course is intended for chemical engineering students. It will introduce quantum theory, atomic and molecular structure, symmetry, computational chemistry, spectroscopy, and statistical thermodynamics. 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; Electronic Spectroscopy; Magnetic Spectroscopy; Boltzmann Distribution Function; Partition Functions; Calculation of Thermodynamic Quantities from Partition Functions.

Text: Ball, D. *Physical Chemistry*, 2nd ed.; Cengage, 2015.

We will cover Chapters 9-18 of the textbook. Some supplemental topics, or enhancements of topics in the textbook, will occasionally be presented. A few topics in the textbook will not be covered. A class schedule will be maintained in the Syllabus section of CourseWeb, and will be updated as needed.

Reference texts: There are many physical chemistry textbooks in the Chemistry Library (Chevron 130): QD 450-801.

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

How the class will be conducted: Given the amount of material we need to go over, lecture periods will need to be devoted mostly to lecture, but we will occasionally devote some time to problem solving. I would be happy to schedule optional problem solving sessions, to help you with the homework.

Final Exam & Examlets: After every two chapters we will have an “examlet”, i.e. an extended quiz. This will help you keep up with the material on a regular basis. The final exam will be take-home, covering Chapters 17 and 18. It will be due at 5:00 pm on Friday, December 13. The final exam period, Wednesday, December 11, 4:00 – 5:50 pm, will be used for a take-home exam clinic, where you can get help on the exam (attendance is optional). The examlets and final exam will focus on problem solving.

There are no make-up examlets, and they can be taken early only for valid reasons. At the discretion of the instructor, the score for a missed examlet will be the average of your other examlet scores. If you have a conflict with an upcoming examlet, please see the instructor. If you had an emergency situation which caused you to miss an examlet, please see the instructor ASAP.

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 examlets.

Projects: Several 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	60% (15% each)
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 examlet 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/>

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