Chemistry 384, Spring Semester 2016:
Introduction to Physical Chemistry II

Professor Warren F. Beck

Revised 23 January 2016: Accessibility section added

Course Description
This course provides an introduction to quantum mechanics and spectroscopy with an emphasis on applications in biochemistry and biophysics. It is intended for B.A-degree Chemistry majors and non-Chemistry majors, such as those in Biochemistry and in health-related fields. The CEM 483/484 sequence is intended for B.S.-degree Chemistry and Chemical Engineering majors.

The course outline is designed to give the student a better understanding of molecular structure and intermolecular forces, especially those in macromolecules. Aspects of statistical mechanics are included so that the concepts of populations in energy levels, temperature, and heat capacity can be discussed.

Instructor and Teaching Assistants
Professor Warren F. Beck: email: beckw@msu.edu; office hours: 3 Chemistry, 4–5 pm after lectures, and additional hours ad libitum or by appointment.
TAs: Soumen Ghosh and Dan Roscioli

Schedule
Lectures: 3:00–3:50 pm MWF, 1415 BPS.

Discussion Section 001: Monday, 11:30 am–12:20 pm, 127 Chemistry.
Discussion Section 002: Tuesday, 11:30 am–12:20 pm, 085 Chemistry.
Discussion Section 003: Tuesday 12:40 pm–1:30 pm, 085 Chemistry.
Discussion Section 004: Monday 12:40 pm–1:30 pm, 085 Chemistry.

The discussion sections begin 25 and 26 January. They will not meet the weeks of 11 January (the first week of the semester), 18 January (MLK day, University holiday), 22 February (first mid-term exam), and 18 April (second mid-term exam).

Practice Test: Wednesday, 10 February 2016, 3:00–3:50 pm, 1415 BPS
Midterm Examination #1: Monday, 22 February 2016, 3:00–3:50 pm, 1415 BPS
Midterm Examination #2: Monday, 18 April 2016, 3:00–3:50 pm, 1415 BPS
Final Examination: Wednesday, 4 May 2016, 3:00–5:00 pm, 1415 BPS
Suggested Textbooks

As the course progresses, a set of lecture notes (slides and outlines) will be posted on Desire to Learn (D2L, https://d2l.msu.edu) in advance of each lecture. The course content is fully presented in the lecture notes, but the student will benefit from additional reading in a formal physical chemistry text that covers quantum mechanics and spectroscopy at an introductory level.

The following texts are suggested as examples:


Readings from Atkins and de Paula, 2e, will be suggested in lecture; this text is used in CEM 383 in the fall semester, so it is generally available.

Outline

1. Principles of Quantum Mechanics
   a. Quantization and wavelike behavior of matter and radiation
   b. Classical Mechanics: harmonic oscillator
   c. Postulates of Quantum Mechanics
   d. Particle-in-a-box problem
   e. Harmonic and anharmonic oscillators
   f. Transition dipole moment and selection rules for optical transitions
   g. Statistical Thermodynamics
   h. Boltzmann distribution
   i. Partition function
   j. Heat capacity and vibrational modes

2. Electronic Structure and Chemical Bonding
   a. Hydrogen atom
   b. Many-electron atoms
   c. Covalent bonding: valence and molecular orbital theories
   d. Diatomic molecules
   e. Polyatomic molecules
   f. Intermolecular forces: hydrogen bonds, van der Waals interactions
   g. Bonding in biological macromolecules

3. Spectroscopy and Applications
   a. Photophysics
   b. Franck-Condon principle and vibronic structure
   c. Two level systems: lasers and protein unfolding
Discussion Sections, Problem Sets, and Homework Problems

The discussion sections will feature in-class exercises as preparation for the problem sets. These exercises will be handed in and graded for on a credit/no-credit/bonus basis.

Problem sets will be assigned for each week that the discussion sections meet. The problem sets will be posted on D2L a week in advance of the due date. They are due at the beginning of lecture on Fridays.

Homework problems will appear, usually daily, in the posted lecture notes. These problems will be due at the beginning of lecture.

Course Grade and Rules

The course grade on the 0.0–4.0 scale will be determined from the final course percentage on an absolute scale, as specified below. The course percentage out of a total of 100% will be calculated as follows: weekly problem sets (10%), practice test and quizzes (10%), daily homework exercises (5%), two mid-term exams (25% each), and final examination (25%). Extra credit questions will be offered on the midterms and quizzes, so there will be more points available than required to obtain the full percentage for that part of the course grade.

The following absolute scale will be used to assign the grades: 4.0 for >88%; 3.5 for >82%; 3.0 for >74%; 2.5 for >68%; 2.0 for >60%; 1.5 for >50%; 1.0 for >40%; and 0.0 for <40%.

Rules and FAQ. Scheduling conflicts should be discussed with the instructor in advance of the midterm exams so that options can be discussed. At the instructor’s discretion, a missed midterm with an approved and documented excuse will be credited using the final exam score on a pro-rated percentage basis.

Because make-up quizzes will not be offered, the lowest two quiz scores will be dropped from the course grade calculation. This rule allows students to miss classes owing to illness and/or travel without suffering a penalty. The student will have to complete all the homework exercises and weekly problem sets; no scores will be dropped for those assignments.

Academic Honesty and Integrity. In this course, the problem sets are intended to be worked out by a student without direct aid from others. Copying of this work from another student’s paper or another source is not permitted, and if detected by one of the TAs or by the instructor, the student will receive a grade of 0 for that assignment. That said, verbal discussion (but not by email or text message, etc.) of how to work problems with other students in the class in a study group is encouraged; each student is responsible for directly performing and writing up all of the calculations, derivations, written discussion, etc., that are turned in for a grade.

Quizzes, midterms, and the final examination are conducted as closed-book, closed-notes exercises unless specified otherwise by the instructor.

Cheating or other academic misconduct will be treated by the instructor as specified in MSU Policies, Regulations, and Ordinances … and by the Office of the MSU Ombudsman: https://www.msu.edu/unit/ombud/academic-integrity/

The student has the right to contest any judgment or penalty grade assigned by the instructor in an academic grievance hearing; see item 6 at the above link.

Accessibility. Michigan State University is committed to providing equal opportunity for participation in all programs, services, and activities. Requests for accommodations by
persons with disabilities may be made by contacting the Resource Center for Persons with Disabilities by phone at 517-884-RCPD or through the web at https://www.rcpd.msu.edu/. Once your eligibility for an accommodation has been determined, you will be issued a verified individual services accommodation ("VISA") form. Please present this form to the instructor at the start of the semester and/or at least two weeks prior to the accommodation date (test, final exam, homework, etc.). Requests received after this date will be honored whenever possible.