

## **Chemistry 384, Spring Semester 2017: Introduction to Physical Chemistry II**

Professor Warren F. Beck

### **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](mailto:beckw@msu.edu);

*office hours:* 3 Chemistry, 4–5 pm after lectures, and additional hours *ad libitum* or by appointment.

TAs: Soumen Ghosh and Jason Gurchiek

### **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:* Wednesday 12:40 pm–1:30 pm, 085 Chemistry.

*Discussion Section 004:* Monday 12:40 pm–1:30 pm, 085 Chemistry.

***The discussion sections begin 23 and 24 January. They will not meet the weeks of 9 January (the first week of the semester), 16 January (MLK day, University holiday), 20 February (first mid-term exam), and 17 April (second mid-term exam).***

*Practice Test #1:* Wednesday, 8 February 2017, 3:00–3:50 pm, 1415 BPS

*Midterm Examination #1:* Monday, 20 February 2017, 3:00–3:50 pm, 1415 BPS

*Practice Test #2:* Wednesday, 5 April 2017, 3:00–3:50 pm, 1415 BPS

*Midterm Examination #2:* Monday, 17 April 2017, 3:00–3:50 pm, 1415 BPS

*Final Examination:* Wednesday, 3 May 2017, 3:00–5:00 pm, 1415 BPS

### **Suggested Textbooks**

Outline materials and lecture notes will be posted on Desire to Learn (D2L, <https://d2l.msu.edu>) in advance of each lecture. 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:

Peter Atkins and Julio de Paula, *Physical Chemistry for the Life Sciences*, W.H. Freeman, New York: 1e, 2006; ISBN: 0-7167-8628-1, or 2e, 2011; ISBN: 978-1-4292-3114-5. (The 2e version was the text for CEM 383, FS16).

Robert J. Silbey, Robert A. Alberty, and Moungi G. Bawendi, *Physical Chemistry*, 4e, Wiley, 2005; ISBN: 9780471215042.

Donald A. McQuarrie and John D. Simon, *Physical Chemistry: A Molecular Approach*, University Science Books, 1997; ISBN: 0935702997.

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

## Quizzes, Discussion Sections and Problem Sets

Quizzes (15 minutes) will be given in lectures on Wednesdays but occasionally on other days. Two practice tests (30 minutes) will be provided a week and a half prior to the midterms.

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.

The discussion sections are intended to help the students with the problem sets. The TAs will often provide some additional coverage of lecture topics.

## 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 (15%), quizzes and practice tests (10%), two mid-term exams (25% each), and final examination (25%).

The following absolute scale will be used to assign the grades: 4.0 for >90%; 3.5 for >83%; 3.0 for >75%; 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 two practice exams are graded and are counted as quizzes.

Quizzes, midterms, and the final examination are conducted as closed-book, closed-notes exercises unless specified otherwise by the instructor. Mobile phones are to be turned off and put away for the duration of the exercise.

**Academic Honesty and Integrity.** In this course, the graded assignments are to be worked out by a student without being aided by others. Copying of work from another student's paper or another source is not permitted; the use of mobile phones for any purpose during a quiz, midterm, or final exam will be treated as academic misconduct. Problems sets may be discussed by study groups, but each student is to turn in work that was written or worked out without copying another student's paper.

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.