

## Physical Chemistry II (CHEM 302)

Spring 2012

Lecture: Tu, Th 10:00AM to 11:15, Cudahy Hall - 202  
Discussion: Tu, Th 11:30AM to 12:20, Flanner Hall - 133

Instructor: Jan Florián  
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Office Hours: Wedn 2:00-3:30 PM and immediately after each class  
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*“Classical Physics did an excellent job accounting for large aggregate states – for the familiar reality that we experience in our everyday lives – but failed to describe the underlying properties of matter and radiation on the atomic level. Quantum Mechanics is an effort to describe this strange yet compelling world in which things are not what they seem to be.”*

-Cass Sacket

*“Chemistry is essentially about bonding of atoms to form molecules. Since a chemical bond is a purely quantum phenomenon, this alone underscores the importance of quantum mechanics to chemistry.”*

-from Physical Chemistry, Keith Laidler, John Meiser, and Brian Sanctuary

*“Physical chemistry is not inherently harder than any other technical subject. It is very mathematical, and students who may have formally satisfied the calculus requirements may still find physical chemistry a challenge because it requires to **apply** the calculus.”*

-from Physical Chemistry, David W. Ball

### Course Objectives

Part 1: Quantum Mechanics and Atomic Structure

1. Understand the basic concepts of quantum mechanics and underlying mathematics
2. Apply quantum mechanics to the study of atomic structure

Part 2: The Chemical Bond

3. Apply quantum mechanics to the study of molecular structure

Part 3: Foundations of Chemical Spectroscopy

4. Understand how light interacts with matter on the molecular level
5. Understand the relationship between quantum mechanics and spectroscopy.

### Required Materials:

1. Ira Levine, Physical Chemistry, McGraw-Hill, 6th Edition
2. iclicker remote control device for in-class response (buy in Loyola or Beck's bookstore or online on iclicker.com (new) or Ebay (used) and register it in class.
3. a non-programmable calculator, capable of scientific notation.

**Recommended books:** Student solutions manual

Applied Mathematics for Physical Chemistry 3<sup>rd</sup> ed. by James R. Barrante

## Grading

Class activity      Maximum number of grading points

|            |                         |
|------------|-------------------------|
| Homework   | 20 pt                   |
| iClicker   | 20 pt                   |
| Exams      | 60 pt (20 pt each exam) |
| Final exam | 40 pt                   |

Grading points for iClicker activity will be calculated from your iClicker % and total exam % using Table 1.  
 Grading points for Homework activity will be calculated from your Homework % and total exam % using Table 1.

**Table 1**

| HW or clicker %/exam % | 0.0  | 5.0 | 10.0 | 15.0 | 20.0 | 25.0 | 30.0 | 35.0 | 40.0 | 45.0 | 50.0 | 55.0 | 60.0 | 65.0 | 70.0 | 75.0 | 80.0 | 85.0 | 90.0 | 95.0 | 100.0 |
|------------------------|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|
| 0.0                    | 0    | 0   | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0     |
| 5.0                    | 0.96 | 1   | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1     |
| 10.0                   | 1.84 | 1.9 | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2    | 2     |
| 15.0                   | 2.64 | 2.8 | 2.9  | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3    | 3     |
| 20.0                   | 3.35 | 3.5 | 3.7  | 3.8  | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4    | 4     |
| 25.0                   | 4    | 4.2 | 4.4  | 4.6  | 4.8  | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5    | 5     |
| 30.0                   | 4.57 | 4.8 | 5    | 5.3  | 5.5  | 5.8  | 6    | 6    | 6    | 6    | 6    | 6    | 6    | 6    | 6    | 6    | 6    | 6    | 6    | 6    | 6     |
| 35.0                   | 5.08 | 5.3 | 5.6  | 5.9  | 6.2  | 6.4  | 6.7  | 7    | 7    | 7    | 7    | 7    | 7    | 7    | 7    | 7    | 7    | 7    | 7    | 7    | 7     |
| 40.0                   | 5.53 | 5.8 | 6.1  | 6.4  | 6.7  | 7    | 7.4  | 7.7  | 8    | 8    | 8    | 8    | 8    | 8    | 8    | 8    | 8    | 8    | 8    | 8    | 8     |
| 45.0                   | 5.93 | 6.2 | 6.5  | 6.9  | 7.2  | 7.5  | 7.9  | 8.3  | 8.7  | 9    | 9    | 9    | 9    | 9    | 9    | 9    | 9    | 9    | 9    | 9    | 9     |
| 50.0                   | 6.28 | 6.6 | 6.9  | 7.3  | 7.6  | 8    | 8.4  | 8.8  | 9.2  | 9.6  | 10   | 10   | 10   | 10   | 10   | 10   | 10   | 10   | 10   | 10   | 10    |
| 55.0                   | 6.59 | 6.9 | 7.2  | 7.6  | 8    | 8.4  | 8.8  | 9.2  | 9.7  | 10   | 11   | 11   | 11   | 11   | 11   | 11   | 11   | 11   | 11   | 11   | 11    |
| 60.0                   | 6.85 | 7.2 | 7.5  | 7.9  | 8.3  | 8.7  | 9.1  | 9.6  | 10   | 11   | 11   | 12   | 12   | 12   | 12   | 12   | 12   | 12   | 12   | 12   | 12    |
| 65.0                   | 7.09 | 7.4 | 7.8  | 8.2  | 8.6  | 9    | 9.4  | 9.9  | 10   | 11   | 11   | 12   | 13   | 13   | 13   | 13   | 13   | 13   | 13   | 13   | 13    |
| 70.0                   | 7.29 | 7.6 | 8    | 8.4  | 8.8  | 9.2  | 9.7  | 10   | 11   | 11   | 12   | 12   | 13   | 13   | 14   | 14   | 14   | 14   | 14   | 14   | 14    |
| 75.0                   | 7.46 | 7.8 | 8.2  | 8.6  | 9    | 9.4  | 9.9  | 10   | 11   | 11   | 12   | 13   | 13   | 14   | 14   | 15   | 15   | 15   | 15   | 15   | 15    |
| 80.0                   | 7.61 | 8   | 8.3  | 8.7  | 9.1  | 9.6  | 10   | 11   | 11   | 12   | 12   | 13   | 13   | 14   | 15   | 15   | 16   | 16   | 16   | 16   | 16    |
| 85.0                   | 7.74 | 8.1 | 8.5  | 8.8  | 9.3  | 9.7  | 10   | 11   | 11   | 12   | 12   | 13   | 14   | 14   | 15   | 16   | 16   | 17   | 17   | 17   | 17    |
| 90.0                   | 7.85 | 8.2 | 8.6  | 9    | 9.4  | 9.8  | 10   | 11   | 11   | 12   | 12   | 13   | 14   | 14   | 15   | 16   | 17   | 17   | 18   | 18   | 18    |
| 95.0                   | 7.94 | 8.3 | 8.7  | 9    | 9.5  | 9.9  | 10   | 11   | 11   | 12   | 13   | 13   | 14   | 14   | 15   | 16   | 17   | 17   | 18   | 19   | 19    |
| 100.0                  | 8.02 | 8.4 | 8.7  | 9.1  | 9.5  | 9.9  | 10   | 11   | 11   | 12   | 13   | 13   | 14   | 15   | 15   | 16   | 17   | 18   | 18   | 19   | 20    |

In the calculation of your **total grading points**, your lowest score will be dropped. If this lowest score includes the final exam, final exam score will be halved. Additional three grading points for mentoring will be awarded after each hourly-exam to each member of the top team, and one point to each member of the second team. Thus, the maximum number of grading points obtainable in the class is 129.

**Letter grades for the class will be assigned according to the following scale (Table 2):**

**Table 2:** Conversion of total grading points to letter grades.

| Earned Grading Points | Letter Grade | Earned Grading Points | Letter Grade |
|-----------------------|--------------|-----------------------|--------------|
| >100                  | A            | 60 – 65               | C            |
| 90 – 100              | A-           | 56 – 60               | C-           |
| 83 – 90               | B+           | 51 – 56               | D+           |
| 76 – 83               | B            | 46 – 51               | D            |
| 70 – 76               | B-           | 46 or less            | F            |
| 65 – 70               | C+           |                       |              |

**Midterm grades:** Midterm grades will be posted on Blackboard after Exam 2. They will be calculated from the two mid-semester exam results, iClicker sessions and homeworks (i.e. maximum of 80 points). Your total points will be multiplied by 120/80 and resulting points will be converted to your midterm letter grade using Table 2.

**Homeworks:** Eight homework assignments, each worth of two or three points will be assigned on Thursday. To receive full credit, a student’s homework has to be submitted in person at the beginning of the next lecture. The homework must also present meaningful steps to solving assigned problems. Late or less than 1/3 completed homeworks will receive zero points.

**Examinations:** If an exam is missed, there will be no make-ups under any circumstances. As mentioned above, the low score for an exam is dropped, so a missed exam would simply be the one dropped. Only non-programmable scientific calculators (TI-30XA) will be allowed during the exam. Students will be able to use pre-prepared hand-written letter-size sheet with formulas of their choice during all exams. Students must follow the seating assignments.

**Ethical Considerations:** *Students will not collaborate on any exams. Students may collaborate on general solution strategy for iClicker and homework problems but each student must present his own solution. Only those materials and devices permitted by the instructor may be used to assist in examinations. Students will not represent the work of others as their own. Identical homeworks will receive zero points. Any student caught cheating during an exam will be reported to the Deans office and will receive zero points for the given exam.*

**Teamwork and Reading Assignments:** In order to understand the material presented during lectures and discussions, it is important to come to the class with good background knowledge. This can be achieved by reading (and thinking about) material in the textbook covered during the semester, reviewing appropriate material from calculus, physics and general chemistry classes, and solving end-of-chapter problems. The reading assignments will be given at the end of each class. Student's knowledge of the material from these assignments will be randomly tested during lectures and discussions using iClicker classroom response system. iClicker questions may also refer to the material presented during lectures. Work together with your classmates; if you don't understand something, someone else may. You will also find that explaining a solution to your classmate will improve your understanding and long-term retention of the material. At any given time, class will be subdivided into teams of three to four students. Joint learning within each team will be encouraged by awarding extra grading points to all members of the two teams that have the best team-average result on each of the three hourly exams during the semester. After each exam, members of the two top teams, the three lowest teams, and any other dysfunctional team will be reshuffled.

#### Schedule

| Date   | Class | Topic                             | Reading           |
|--------|-------|-----------------------------------|-------------------|
| 17-Jan | 1     | Pre-Schrodinger QM (17.1 - 17.5)  | n/a               |
| 19-Jan | 2     | QM Formalism I                    | 17.1 - 17.5       |
| 24-Jan | 3     | QM Formalism II                   | 17.6 - 17.7       |
| 26-Jan | 4     | Particle in a box                 | 17.8 - 17.9       |
| 31-Jan | 5     | Degeneracy, Operators             | 17.10 - 17.11     |
| 2-Feb  | 6     | Harmonic oscillator, Reduced mass | 17.12 - 17.13     |
| 7-Feb  | 7     | Rigid rotor, Numerical methods    | 17.14 - 17.15     |
| 9-Feb  | 8     | QM Formalism III                  | 17.16 - 17.17     |
| 14-Feb | 9     | Exam 1                            |                   |
| 16-Feb | 10    | One-electron atoms                | 18.1 - 18.3       |
| 21-Feb | 11    | Orbital and spin magnetism        | 18.4 - 18.5       |
| 23-Feb | 12    | Two-electron atoms                | 18.6 - 18.7       |
| 27-Feb | 13    | Many-electron atoms I             | 18.8              |
| 1-Mar  | 14    | Many electron atoms II            | 18.9 - 18.10      |
| 6-Mar  |       | Spring break                      |                   |
| 8-Mar  |       | Spring break                      |                   |
| 13-Mar | 15    | Exam 2                            |                   |
| 15-Mar | 16    | Chemical bonding I                | 19.1              |
| 20-Mar | 17    | Chemical bonding II               | 19.2 - 19.3       |
| 22-Mar | 18    | Molecular orbitals                | 19.4 - 19.5       |
| 27-Mar | 19    | Computational Chemistry I         | 19.7 - 19.9       |
| 29-Mar | 20    | Computational Chemistry II        | 19.10 - 19.12     |
| 3-Apr  | 21    | Computational Chemistry III       | 19.13 - 19.15     |
| 5-Apr  | 22    | Introduction to spectroscopy I    | 20.1 - 20.2       |
| 10-Apr | 23    | Introduction to spectroscopy II   | 20.3 - 20.4       |
| 12-Apr | 24    | Molecular Symmetry                | 20.5, 20.16       |
| 17-Apr | 25    | Exam 3                            |                   |
| 19-Apr | 26    | Vibrational spectroscopy          | 20.8 - 20.10      |
| 24-Apr | 27    | Electronic spectroscopy           | 20.11, 20.14-15   |
| 26-Apr | 28    | Magnetic resonance spectroscopy   | 20.12 - 13, 20.17 |
| 1-May  |       | Final Exam, Cudahy 202, 1 pm      |                   |

Note: The instructor reserves the right to make changes to the schedule. Any changes to exam dates will be announced in class and on blackboard.