# Chem 562: Physical Chemistry

Spring 2019

**Instructors**

Prof. Etienne Garand (egarand@wisc.edu)
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Office Hours: Wednesdays 3-4pm in Chem 8305F
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Office Hours: Thursdays 3-4pm in Chem 8305F

**Meeting Time and Location**

Lecture: MWF 8:50-9:40PM in 1315 Chemistry Building

Discussion 401: T 8:50-9:40AM in B379 Chemistry Building
Discussion 402: T 9:55-10:45AM in B379 Chemistry Building
Discussion 403: T 2:25-3:15PM in 2333 Sterling Hall
Discussion 404: T 3:30-4:20PM in 2333 Sterling Hall

**Course Credit Information**

The credit standard for this course is met by an expectation of a total of 135 hours of student engagement with the course learning activities (at least 45 hours per credit), which include regularly scheduled meeting times [three times weekly for 50 minutes lecture and weekly for 50 minutes discussion section], reading, problem sets, studying, etc.

**Official Course Description (as published in the catalog)**

Molecular theory: quantum chemistry, molecular structure and spectra, statistical mechanics, selected topics in the molecular theory of matter in bulk.

**Official Requisites (as published in the catalog)**

Chem 561 or 565 or ChE 211; Physics 202 or 208

**Course Designations and Attributes (from catalog)**

Advanced level; physical science breadth; counts as L&S credit;

**Learning outcomes**

This course discusses the microscopic view of matter and chemical phenomena using the tools of quantum mechanics and statistical thermodynamic. The overall goal is to provide the physical and mathematical underpinnings of a molecular description of physical and chemical properties.

1. Describe fundamental quantum mechanics concepts, including operators, wavefunctions, and uncertainty principle.
2. Use quantum chemistry models to describe translational, rotational, and vibrational motion of particles, the microscopic details of atomic and molecular structures, and the basis of rotational, vibrational and electronic spectroscopies.
3. Apply quantum chemistry and statistical thermodynamic models to describe bulk thermodynamic properties, chemical equilibrium and chemical reaction dynamics.

**Textbook**

The class material closely follows Physical Chemistry (11$^{th}$ edition) by Atkins, DePaula and Keeler (Oxford University Press) The book is not required for the class but is strongly recommended. The chapter layout and material are very similar in the previous 9$^{th}$ and 10$^{th}$ editions

**Discussion**

Your teaching assistant will meet with you for a discussion section on Tuesdays. Sections 401 (8:50 am) 402 (9:55 am) and 403 (2:25 pm) meet in Room B357 and section 404 (3:30pm) meets in 2311. This meeting is to discuss material from the lectures, the text and the assigned problems.

**Problem Sets**

Doing problem sets is essential to mastering the material in this course. There will be a problem set most weeks except those weeks that follow exams. There are 11 problem sets in total but we will drop your lowest score. The problem sets are due at the beginning of the class period on Friday unless otherwise noted. The due dates and PDF files of the problem sets are on the class website. You are free to work with others on the problem sets and will probably find it useful, but you must write up your own answers.

**Exams**

There will be three exams as noted on the course outline.
**Exam #1:** Monday March 4, during lecture
**Exam #2:** Monday April 8, during lecture
**Exam #3:** Monday May 6, 7:45am, location TBD

**Grades**

Grades will be determined by an equal weighting of each exam and the problem sets.
Problem Sets (Best 10 of 11): 25%
Exam #1 (March 4): 25%
Exam #2 (April 8): 25%
Exam #3 (May 6): 25%

**Course Outline**

| W | L | Date | PS | Topic | Atkins 9th e | Atkins 11th e |
|---|---|---|---|---|---|---|
| 1 | 1 | Jan. 23 W | | Classical mechanics review | F. Info 7.1 | |
| | 2 | Jan. 25 F | | Origins of quantum mechanics | 7.1-7.2 | 7A |
| 2 | 3 | Jan. 28 M | | Schrodinger equation | 7.3 | 7B.1 |
| | 4 | Jan. 30 W | | Wavefunctions | 7.4 | 7B.2 |
| | 5 | Feb. 1 F | PS #1 | Operators and observables | 7.5 | 7C.1-2 |
| 3 | 6 | Feb. 4 M | | Uncertainty principle | 7.6 | 7C.3-4 |
| | 7 | Feb. 6 W | | Translation: particle in a 1-D box | 8.1, 8.3 | 7D.1-2 |
| | 8 | Feb. 8 F | PS #2 | Particle in a 2-D box | 8.2 | 7D.3-4 |
| 4 | 9 | Feb. 11 M | | Vibrations: Harmonic oscillator | 8.4-8.5 | 7E |
| | 10 | Feb. 13 W | | Rotation: Particle on a ring | 8.6 | 7F.1 |
| | 11 | Feb. 15 F | PS #3 | Particle on a sphere and spin | 8.7-8.8 | 7F.2 |
| 5 | 12 | Feb. 18 M | | Rotations of molecules | 12.3-12.4 | 11B.1 |
| | 13 | Feb. 20 W | | Rotational spectroscopy | 12.5 | 11B.2 |
| | 14 | Feb. 22 F | PS #4 | Molecular vibrations | 12.8-12.10 | 11C.1, 11C.3 |
| 6 | 15 | Feb. 25 M | | Ro-vibrational spectroscopy | 12.11 | 11C.2, 11C.4 |
| | 16 | Feb. 27 W | | Vibrations of polyatomic molecules | 12.13-12.14 | 11D.1-2 |
| | 17 | Mar. 1 F | PS #5 | Atomic structure: Hydrogen atom | 9.1 | 8A.1 |
| 7 | | **Mar. 4 M** | | **Exam #1 (Lectures 1-16)** | | |
| | 18 | Mar. 6 W | | Hydrogenic orbitals | 9.2-9.3 | 8A.2, 8C.1 |
| | 19 | Mar. 8 F | | Multielectron atoms | 9.4 | 8B.1-2 |
| 8 | 20 | Mar. 11 M | | Multielectron atoms | 9.4-9.5 | 8B.3-4 |
| | 21 | Mar. 13 W | | Singlets and triplets | 9.8 | 8C.2a |
| | 22 | Mar. 15 F | PS #6 | Valence bond theory | 10.1-10.2 | 9A.1, 9A.3 |
| 9 | | Mar 18-22 | | Spring Recess | | |
| 10 | 23 | Mar. 25 M | | Molecular orbital theory | 10.3 | 9B.1 |
| | 24 | Mar. 27 W | | Homonuclear diatomic molecules | 10.4 | 9C.1 |
| | 25 | Mar. 29 F | PS #7 | Heteronuclear diatomic molecules | 10.5 | 9D.1 |
| 11 | 26 | Apr. 1 M | | Polyatomic molecules | 10.6-10.7 | 9D.2, 9E.3 |
| | 27 | Apr. 3 W | | Electronic spectroscopy | 13.2-13.3 | 11F.1c |
| | 28 | Apr. 5 F | PS #8 | Photochemistry | 13.4-13.5 | 11G |
| 12 | | **Apr. 8 M** | | **Exam #2 (Lectures 17-28)** | | |
| | 29 | Apr. 10 W | | Configuration and weight | 15.1 | 13A |
| | 30 | Apr. 12 F | | Molecular partition functions | 15.2 | 13B.1 |
| 13 | 31 | Apr. 15 M | | Molecular partition functions | 16.2 | 13B.2 |
| | 32 | Apr. 17 W | | Internal energy | 15.3 | 13C |
| | 33 | Apr. 19 F | PS #9 | Entropy | 15.4 | 13E.2 |
| 14 | 34 | Apr. 22 M | | Canonical partition function | 15.5-15.7 | 13D.1-3 |
| | 35 | Apr. 24 W | | Thermodynamic functions | 16.3-16.4 | 13E.1, 13F.1 |
| | 36 | Apr. 26 F | PS #10 | Equilibrium | 16.8 | 13F.2 |
| 15 | 37 | Apr. 29 M | | Reactive encounters | 22.1 | 18A.1 |
| | 38 | May 1 W | | Diffusion controlled reactions | 22.2 | 18B.1 |
| | 39 | May 3 F | PS #11 | Activated complex theory | 22.4-22.5 | 18C.1-2 |
| 16 | | **May 6 M** | | **Exam#3 7:45AM (Lectures 29-39)** | | |