**CHEM 336: Physical Chemistry III**

**Dr. Alisa Krishtal krishtal@njit.edu**

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| Lectures: | Monday | 10:00 am - 11:25 am | FMH 310 |
| | Wednesday | 10:00 am - 11:25 am | FMH 310 |
| Recitation/Tutoring | Wednesday | 2:30 pm - 3:55 pm | TBD |
| Office Hours: | Monday | 02:00 pm - 04:00 pm | Tier 323B |
| | Wednesday | 01:00 pm - 02:30 pm | Tier 323B |
| | Friday | 02:00 pm - 04:00 pm | Tier 323B |

## COURSE REQUIREMENTS

- **Required Textbook:** "Physical Chemistry: Thermodynamics, Structure, and Change" by Peter Atkins and Julio de Paula, **10th edition**, Freeman. ISBN-10: 1-4292-9019-6; ISBN-13: 978-1-4292-9019-7. Student Solution Manual is strongly recommended.
- **Prerequisite courses:** Chem 235 with grade C or better.
- **Prerequisite knowledge:** Functions of two and several variables, partial derivatives, integrals, differential equations, classical mechanics, electricity and magnetism, basic chemical principles.

**LECTURES:** Students are expected to read the specified textbook material **before** coming to class. The lectures will consist out of in depth discussion of the material and solving of exercises and problems. Students are required to bring the textbook to each lecture.

**CLASS PARTICIPATION**: A high level of active participation is expected, including participating in discussions and presenting homework problems on the board, and will be part of the final grade.

**HOMEWORK:** Homework will be assigned on a weekly basis depending on the material covered in class and will be due by the next week's lecture. The homework will be assigned from the end of chapter exercises and problems in the book. If you're using an older edition of the book, the numbering of the exercises and problems will be different and it will be your responsibility to come see me to find out the correct numbering in your edition. At the homework due date, all students must be prepared to present any homework exercise on the board. Homework will be collected by the end of the lecture.

**QUIZZES:** Quizzes might be given during the lectures without prior announcement and will be based on the homework. Eventual quizzes grades will count towards the homework grade. All quizzes are **open book** and **closed notes**. Only bound textbooks are allowed: no printouts of e-books or copies of chapters are allowed. No electronic devices are allowed during quizzes except for a non-graphical calculator.

**EXAMS:** There will be 2 exams as listed in the Tentative Course Schedule and a final exam at the end of the course. All exams are **open book** and **closed notes**. Material covered on exams is **cumulative**. Only bound textbooks are allowed: no printouts of ebooks or copies of chapters. No electronic devices are allowed during exams except for a non-graphical calculator.

**COURSE GRADING:**

- Exam 1: 20%
- Exam 2: 20 %
- Final exam: 30%
- Homework: 20%
- Class participation: 10%

**GRADING POLICY:** Exact grade cutoffs will be determined on a semester-by-semester basis, depending on how the class performs. There is no requirement for any A's or any F's to be awarded during any particular semester. Information on individual performance and projected grade will be given during the semester after each exam and at student's request.

**MISSING CLASS:** All excuses must be approved by the Dean of Students due to privacy reasons. Missing a quiz or exam without an approved excuse will result in a zero grade. A make-up quiz may be available at the instructor's discretion.

**MOODLE and EMAIL:** There is a course Moodle site that will include resources and updates of importance to this course, including homework assignments, due dates, exam dates and change of syllabus. Please check it frequently, and also make sure to check or forward your NJIT email in order to receive important announcements. It remains the student's responsibility to stay up to date on any changes.

# Tentative Course Schedule

The schedule is purely tentative and subject to change depending on our progress in class, including exam dates and material covered on exams. It remains the student's responsibility to stay up to date on any changes.

| Date | Topic |
|---|---|
| 01/18 | *Chapter 7: Introduction to Quantum Chemistry*<br>7A: Origins of Quantum Chemistry |
| 01/23 | 7B: Dynamics of microscopic systems |
| 01/25 | 7C: The principles of quantum theory |
| 01/30 | 7C: The principles of quantum theory |
| 02/01 | *Chapter 8: The quantum theory of motion*<br>8A: Translation |
| 02/06 | 8A: Translation |
| 02/08 | 8B: Vibrational motion |
| 02/13 | 8C: Rotational motion |
| 02/15 | 8C: Rotational motion |
| 02/20 | **Exam 1:** Chapters 7 and 8 |
| 02/22 | *Chapter 9: Atomic structure and spectra*<br>9A: Hydrogenic atoms |
| 02/27 | 9A: Hydrogenic atoms |
| 03/01 | 9B: Many-electron atoms |
| 03/06 | 9C: Atomic spectra |
| 03/08 | 9C: Atomic spectra |
| 03/20 | *Chapter 10: Molecular Structure*<br>10A: Valence Bond Theory<br>10B: Principles of molecular orbital theory |
| 03/22 | 10C: Homonuclear diatomic molecules |
| 03/27 | 10D: Heteronuclear diatomic molecules |
| 03/29 | 10E: Polyatomic molecules |
| 04/03 | **Exam 2: Chapters 9 and 10** |
| 04/05 | *Chapter 12: Rotational and vibrational spectra*<br>12A: General features of molecular spectroscopy<br>12B: Molecular rotation |
| 04/10 | 12B: Molecular rotation |
| 04/12 | 12C: Rotational Spectroscopy |
| 04/17 | 12D: Vibrational spectroscopy of diatomic molecules |
| 04/19 | 12E: Vibrational spectroscopy of polyatomic molecules |
| 04/24 | *Chapter 13: Electronic transitions*<br>13A: Electronic spectra |
| 04/26 | 13B: Decay of excited states |
| 05/01 | Review |
| 05/05-11 | **Final exam, Chapters 7-10, 12-13** |

# Recommended exercises and problems

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|---|---|---|
| Chapter 7A | Exercises | 7A.1, 7A.2, 7A.3, 7A.5, 7A.6, 7A.7, 7A.8, 7A.9, 7A.10, 7A.11 |
| | Problems | 7A.1, 7A.2, 7A.6 |
| Chapter 7B | Exercises | 7B.1, 7B.2, 7B.3, 7B.4, 7B.5 |
| | Problems | 7B.1, 7B.2, 7B.3, 7B.5, 7B.7 |
| Chapter 7C | Exercises | 7C.1, 7C.2, 7C.3, 7C.4, 7C.5, 7C.6, 7C.7, 7C.8, 7C.9 |
| | Problems | 7C.1, 7C.2, 7C.3, 7C.4, 7C.5, 7C.7, 7C.8, 7C.9, 7C.15, 7C.16 |
| Chapter 8A | Exercises | 8A.1, 8A.2, 8A.3, 8A.4, 8A.5, 8A.6, 8A.8, 8A.10 |
| | Problems | 8A.1, 8A.2, 8A.3, 8A.8 |
| Chapter 8B | Exercises | 8B.1, 8B.2, 8B.3, 8B.4, 8B.6, 8B.7, 8B.8 |
| | Problems | 8B.1, 8B.2, 8B.4, 8B.5, 8B.6, 8B.8 |
| Chapter 8C | Exercises | 8C.1, 8C.2, 8C.3, 8C.4, 8C.5, 8C.6, 8C.7 |
| | Problems | 8C.1, 8C.3, 8C.5, 8C.6, 8C.8, 8C.9, 8C.11 |
| Chapter 9A | Exercises | 9A.1, 9A.2, 9A.3, 9A.4, 9A.5, 9A.6, 9A.7, 9A.8, 9A.9, |
| | Problems | 9A.1, 9A.2, 9A.4, 9A.5, 9A.7, 9A.11 |
| Chapter 9B | Exercises | 9B.1 |
| | Problems | 9B.1, 9B.2 |
| Chapter 9C | Exercises | 9C.1, 9C.2, 9C.3, 9C.4, 9C.5, 9C.7, 9C.8, 9C.9, 9C.10, 9C.11, 9C.12 |
| | Problems | 9C.1, 9C.2, 9C.3, 9C.4, 9C.7 |
| Chapter 10A | Exercises | 10A.1, 10A.2, 10A.3, 10A.5, 10A.6 |
| | Problems | |
| Chapter 10B | Exercises | 10B.1, 10B.2 |
| | Problems | 10B.1, 10B.3 |
| Chapter 10C | Exercises | 10C.1, 10C.2, 10C.3, 10C.4, 10C.5, 10C.6 |
| | Problems | 10C.3, 10C.4 |
| Chapter 10D | Exercises | 10D.1, 10D.2, 10D.3, 10D.5, 10D.6, 10D.7 |
| | Problems | 10D.2 |
| Chapter 10E | Exercises | 10E.1, 10E.2, 10E.3, 10E.4 |
| | Problems | 10E.1 |
| Chapter 12A | Exercises | 12A.1, 12A.2, 12A.3, 12A.4, 12A.6, 12A.8 |
| | Problems | 12A.1, 12A.2, 12A.3, 12A.4 |
| Chapter 12B | Exercises | 12B.1, 12B.3, 12B.5 |
| | Problems | 12B.1, 12B.2 |
| Chapter 12C | Exercises | 12C.1, 12C.2, 12C.3, 12C.4, 12C.5, 12C.6, 12C.7, 12C.8 |
| | Problems | 12C.1, 12C.3, 12C.9 |
| Chapter 12D | Exercises | 12D.1, 12D.2, 12D.3, 12D.4, 12D.5, 12D.6 |
| | Problems | 12D.1, 12D.7, 12D.11, 12D.14, 12D.15 |
| Chapter 12E | Exercises | 12E.1, 12E.2, 12E.3, 12E.4, 12E.5, 12E.6 |
| | Problems | |
| Chapter 13A | Exercises | 13A.1, 13A.2, 13A.3, 13A.4 |
| | Problems | |
| Chapter 13B | Exercises | |
| | Problems | |

# Learning Outcomes

At the end of the course, the student will be able to

- Describe the concept of energy quantization and wave-particle duality of light and matter
- Discuss differences and similarities between classical and quantum chemical models
- Construct the Schrödinger equation for simple systems
- Normalize a wave function and calculate the probability density of a system in a region
- Construct quantum chemical operators and determine expectation values of observables
- Describe the solution of the Schrödinger equation for a free motion in one dimension and confined motion in one and two dimensions, and calculate their properties.
- Use the separation of variables technique
- Describe the solution of the Schrödinger equation for a harmonic oscillator and calculate it's properties.
- Describe the solution of the Schrödinger equation for a particle on a ring and particle on a sphere and calculate their properties.
- Describe the solutions of the Schrödinger equation for hydrogenic atoms and their properties: quantum numbers, orbital energies, classification in shells
- Construct a wave function for a many-electron atom using the orbital approximation
- Interpret atomic spectra of hydrogenic atoms and complex atoms using selection rules and assign term symbols to electronic states of atoms
- Explain the concept of hybridization and molecular orbital theory
- Assign ground state electron configurations to homo- and heteronuclear diatomic molecules
- Use the variation principle to calculate energies of heteronuclear diatomic molecules
- Use the Hückel approximation to calculate the $\pi$-electron binding energy in aromatic molecules.
- Explain the fundamental concepts of absorption and emission spectra
- Calculate moments of inertia of simple molecules and classify them as rotors
- Interpret microwave and Raman rotation spectra of molecules using selection rules
- Interpret IR-spectra of diatomic and polyatomic molecules using selection rules
- Assign term symbols to electronic states of diatomic molecules
- Interpret electronic spectra of molecules using selection rules
- Explain the fluorescence and phosphorescence decay mechanisms