

# **Course ID and Title:** CHEM 431 – Physical Chemistry II: Quantum Mechanics **Units:** 4 **Term:** Spring 2025

Lectures: Mon, Wed, Fri – 11:00-11:50 am Location: ZHS 252

**Discussion:** Fri – 1:00-2:50 pm (problem solving practice led by TA) **Location:** KAP 163

Instructor: Prof. Vadim Cherezov Office: MCB 318 Office Hours: Contact Info: E-mail: <u>cherezov@usc.edu</u>; Phone: 213-379-3613

Teaching Assistant: TBD Office Hours: Contact Info:

# **Course Description**

This course focuses on quantum mechanics as the foundation of atomic and molecular physics, chemical structure and reactivity, and spectroscopy. Students will become aware of the *fundamental physical principles* that form a unified base for understanding chemical and physical properties of matter. Selected topics from Part Two and Part Four of Silbey, Alberty, Bawendi textbook: Quantum Mechanics (Ch. 9); Atomic Structure (Ch. 10); Molecular Structure (Ch. 11); Symmetry (Ch. 12); Rotational and Vibrational Spectroscopy (Ch. 13); Electronic Spectroscopy (Ch. 14); Electric and Magnetic Properties of Molecules (Ch. 22), and Solid State (Ch. 23).

# **Learning Objectives**

By the end of this course, students will be able to:

- Define and explain the fundamental principles of quantum mechanics, including wave-particle duality, the superposition principle, and the uncertainty principle.
- Analyze wavefunctions and explain their significance in quantum mechanics.
- Solve the Schrödinger equation for simple quantum mechanical systems.
- Apply Variational Method and Perturbation theory to more complex quantum mechanical problem.
- Understand the origin of quantization and its application to describe atomic structure.
- Derive atomic and molecular term symbols and use them to describe spectroscopic transitions.
- Classify spectroscopic transitions for atom and molecules as electronic, vibrational, and rotational and derive atomic and molecular properties from specific spectroscopic measurements.

Prerequisite(s): Phys 152

# **Course Notes**

This is a Letter grading course. All information and materials for the course including lecture notes and homework assignments will be available on Brightspace. Lectures will be recorded with Zoom.

# **Required Readings and Supplementary Materials**

Physical Chemistry, by R. J. Silbey, R. A. Alberty, and M. G. Bawendi, 4<sup>th</sup> Edition (John Wiley & Sons, 2005).

# **Optional Readings and Supplementary Materials**

*Physical Chemistry, a Molecular Approach* by D. A. McQuarrie and J. D. Simon *Physical Chemistry* by P. Atkins, J. de Paula and J. Keeler

# **Description and Assessment of Assignments**

Exams and Quizzes:

- There will be 15 min quizzes (a total of 8 throughout the semester) given during Discussion sessions that will count toward the final grade. At the end, two lowest quiz scores may be dropped.
- There will be **2 midterm exams** (50 min each) given during regular class hours. Each of the midterm exams will include the material covered up to that point from the previous midterm exam.
- At the end of the semester, there will be a **comprehensive final exam** (100 min) covering the whole course.
- All quizzes and some exams will be closed-book.
- All exam dates are *final*, there will be no make-up exams except for emergency situations.

## Homework:

- Homework assignments will be posted on Brightspace.
- In addition to regular problems, Homework will contain more challenging bonus problems for extra credit.
- All Homework assignments must be uploaded on time to Brightspace as pdf files. Adobe Scan app is recommended for taking photos of your work and converting to pdf.
- All Homework will be graded and count toward the final grade.
- Any questions regarding the Homework grades should be resolved within a week of receiving the grade.
- Late returns will be accepted with a penalty of 5 points per each day beyond the deadline.

# **Course Policies and Participation**

- Full attendance and active participation in all lectures and discussion are expected.
- Reading assignments from the textbook must be completed *before* each lecture.
- BOTH lecture notes and the textbook should be studied as they do not duplicate each another.
- A zero score will be assigned if an exam/quiz is missed without a legitimate excuse or a homework assignment is not turned in 10 days past the deadline.
- Individuals with excused absences will receive special consideration at the end of the semester. Absences will be excused based on official university policy. All excuses will be verified.
- An incomplete grade (IN) will be assigned when work is not completed because of documented illness or other "emergency" occurring after the twelfth week of the semester.

# **Grading Breakdown**

The final grade will be determined based on the cumulative weighed average score using the grading scale below.

Homework: 15% Quizzes: 15% Midterm exams: 40% Final exam: 30%

# **Grading Scale**

| Letter grade |         |
|--------------|---------|
| А            | 94-100% |
| A-           | 88-93%  |
| B+           | 82-87%  |
| В            | 75-81%  |
| B-           | 69-74%  |
| C+           | 63-68%  |
| С            | 56-62%  |
| C-           | 50-55%  |
| D            | 31-49%  |
| F            | <30%    |

# **Grading Timeline**

All assignments will be graded by TA and verified by the course instructor generally within 7-10 days passed the assignment deadline.

# **Academic Integrity**

The University of Southern California is foremost a learning community committed to fostering successful scholars and researchers dedicated to the pursuit of knowledge and the transmission of ideas. Academic misconduct is in contrast to the university's mission to educate students through a broad array of first-rank academic, professional, and extracurricular programs and includes any act of dishonesty in the submission of academic work (either in draft or final form).

This course will follow the expectations for academic integrity as stated in the <u>USC Student Handbook</u>. All students are expected to submit assignments that are original work and prepared specifically for the course/section in this academic term. You may not submit work written by others or "recycle" work prepared for other courses without obtaining written permission from the instructor(s). Students suspected of engaging in academic misconduct will be reported to the Office of Academic Integrity.

Other violations of academic misconduct include, but are not limited to, cheating, plagiarism, fabrication (e.g., falsifying data), knowingly assisting others in acts of academic dishonesty, and any act that gains or is intended to gain an unfair academic advantage.

Academic dishonesty has a far-reaching impact and is considered a serious offense against the university. Violations will result in a grade penalty, such as a failing grade on the assignment or in the course, and disciplinary action from the university itself, such as suspension or even expulsion.

For more information about academic integrity see the <u>student handbook</u> or the <u>Office of Academic</u> <u>Integrity's website</u>, and university policies on <u>Research and Scholarship Misconduct</u>.

Please ask your instructor if you are unsure what constitutes unauthorized assistance on an exam or assignment or what information requires citation and/or attribution.

# Policy for the use of AI Generators

In this course, the use of artificial intelligence (AI)-powered programs to help you with Homework assignments is allowed. However, it is essential to be aware that AI text generation tools may present incorrect information, biased responses, and incomplete analyses; thus they are not yet prepared to produce text that meets the standards of this course. To adhere to our university values, you must cite any AI-generated material (e.g., text, images, etc.) included or referenced in your work and provide the prompts used to generate the content. Using an AI tool to generate content without proper attribution will be treated as plagiarism and reported to the Office of Academic Integrity.

## **Course Content Distribution and Synchronous Session Recordings Policies**

USC has policies that prohibit recording and distribution of any synchronous and asynchronous course content outside of the learning environment.

Recording a university class without the express permission of the instructor and announcement to the class, or unless conducted pursuant to an Office of Student Accessibility Services (OSAS) accommodation. Recording can inhibit free discussion in the future, and thus infringe on the academic freedom of other students as well as the instructor. (Living our Unifying Values: The USC Student Handbook, page 13).

Distribution or use of notes, recordings, exams, or other intellectual property, based on university classes or lectures without the express permission of the instructor for purposes other than individual or group study. This includes but is not limited to providing materials for distribution by services publishing course materials. This restriction on unauthorized use also applies to all information, which had been distributed to students or in any way had been displayed for use in relationship to the class, whether obtained in class, via email, on the internet, or via any other media. (Living our Unifying Values: The USC Student Handbook, page 13).

# **Course Evaluations**

Course evaluation occurs at the end of the semester university-wide. It is an important review of students' experience in the class. Learning Experience Evaluations are your opportunity to provide feedback to your instructor. USC and its faculty take these evaluations very seriously, as they provide valuable information that faculty and schools can use to improve teaching. It is important to remember that the learning process is collaborative and requires significant effort from the instructor, individual students, and the class as a whole. Please provide a thoughtful assessment of their experience, as well as of their own effort, with comments focused on specific aspects of instruction or the course. Comments on personal characteristics of the instructor are not appropriate and will not be considered. Evaluations should be completed individually with no undue influence by either a student or instructor. Should any inappropriate behavior occur, it will be reported to the Office of Institutional Research.

# **Tentative Course Schedule**

| Week    | Date        | Topics  | Reading<br>assignment (SAB) |
|---------|-------------|---|-----------------------------|
| 1       | 1/13        | Introduction to the course. Math review.  |                             |
|         | 1/15        | Classical mechanics: a deterministic theory. Failures of classical mechanics.                                     | 9.1                         |
|         | 1/17        | The wave-particle duality. The de Broglie wavelength. The Heisenberg Uncertainty Principle. The wavefunction.     | 9.1 - 9.3                   |
| 2       | 1/20        | MLK day – no class  |                             |
|         | 1/22        | The time-dependent Schrödinger equation. Separation of time dependence.<br>Time-independent Schrödinger equation. | 9.14, 9.3                   |
|         | 1/24        | Particle in a 1D box: guantization of energy, nodes of wavefunction.  | 9.6                         |
| 3       | 1/27        | Particle in a 2-D and 3-D box. Degeneracy. Quantum dots. Tunneling. STM.  | 9.7. 9.15                   |
| -       | 1/29        | Operators, Physical observables, Eigenfunctions and eigenvalues.  | 9.4. 9.5. 9.13              |
|         | 1/31        | Commutators, Generalized uncertainty principle. Hermitian operators.  | 9.8. 9.4                    |
| 4       | 2/3         | The superposition principle.  | 9.5                         |
|         | 2/5         | Classical harmonic oscillator. Vibrations of molecules. Quantum mechanical harmonic oscillator.                   | 9.9, 9.10                   |
|         | 2/7         | Operator algebra for harmonic oscillator. Lowering and raising operators.   | handout                     |
| 5       | 2/10        | Rotational motion in 2D: particle on a ring. Rigid rotor.   | 9.11                        |
|         | 2/12        | Rotational motion in 3D: angular momentum.  | 9.12                        |
|         | 2/14        | Generalized angular momentum: operator algebra.   | handout                     |
| 6       | 2/17        | Presidents' Day – no class  |                             |
|         | 2/19        | Part I review, Q&A session.   |                             |
|         | 2/21        | Midterm Exam I  |                             |
| 7       | 2/24        | Hydrogen atom: the Schrödinger equation, separation of variables.   | 10.1                        |
|         | 2/26        | Hydrogen atom: Atomic units, energy levels, spectra.  | 10.1, 10.2, 10.15           |
|         | 2/28        | Hydrogen atom: wavefunctions and atomic orbitals, expectation values of   | 10.3, 10.4                  |
| 0       | 2/2         | Variational Mathed Halium atom  | 10 6 10 7                   |
| 0       | 3/3         | Variational Metriou. Helium atom.   | 10.6, 10.7                  |
|         | 3/5         | Electron spin. Pauli Exclusion Principle.   |                             |
| 0       | 2/10        | Angular momentum of multi-electron atoms  | 10.10, 10.11                |
| 9       | 2/12        | Atomic term symbols   | 10.12                       |
|         | 2/14        | Atomic construction symposis.   | 10.15                       |
|         | 5/14        | Atomic spectroscopy. symmetry and selection rules.  | 10.14                       |
|         | 3/16-<br>23 | Spring break  |                             |
| 10      | 3/24        | Quantum Chemistry. The mean field approximation and SCF Hartree-Fock  | 10.9                        |
|         | 3/26        | Diatomic molecules: the Born-Onnenheimer Approximation  | 11 1                        |
|         | 3/28        | The hydrogen molecular ion $H_2^+$ Multielectron diatomics  |                             |
| 11      | 3/20        | Flectron configuration of homonuclear diatomics. Molecular terms symbols  | 11 5                        |
|         | 4/2         | Part II review O&A session  | 11.5                        |
|         | 4/4         | Midterm Fxam II   |                             |
| 12      | 4/7         | Polyatomic molecules: Valence bond method   | 11.6                        |
| <u></u> | 4/9         | Polyatomic molecules: Huckel's Molecular Orbital theory   | 11 7 11 10                  |
|         | 4/11        | The hand theory of solids: metals, semiconductors, insulators   | handout                     |
| 12      | 7/11        | Commente energetione commente elemente e sistemente.  |                             |
| 13      | 4/14        | Symmetry operations, symmetry elements, point groups.   | 12.1-12.5                   |
|         | 4/10        | Group theory, polarity, chirality.  | 12.0, 12./                  |
| 1       | 4/18        | inne-independent perturbation theory.   | nandout                     |

| 14 | 4/21 | Time-independent perturbation theory: examples.                                   | handout          |
|----|------|---|------------------|
|    | 4/23 | Spectroscopy: an introduction. Einstein coefficients. Lasers.                     | 13.1, 13.2, 14.9 |
|    | 4/25 | Molecular spectroscopy. Rotational spectra of diatomics and polyatomic molecules. | 13.3, 13.4       |
| 15 | 4/28 | Vibration and vibration-rotation spectra of diatomics.                            | 13.6, 13.7       |
|    | 4/30 | Vibrations of polyatomic molecules. Normal modes. Raman spectroscopy              | 13.8, 13.9       |
|    | 5/2  | Final review, Q&A session.  |                  |
|    |      |   |                  |
|    | 5/7  | Final Exam 11:00 am – 1:00 pm   |                  |

# Statement on University Academic and Support Systems

### **Students and Disability Accommodations:**

USC welcomes students with disabilities into all of the University's educational programs. <u>The Office of</u> <u>Student Accessibility Services</u> (OSAS) is responsible for the determination of appropriate accommodations for students who encounter disability-related barriers. Once a student has completed the OSAS process (registration, initial appointment, and submitted documentation) and accommodations are determined to be reasonable and appropriate, a Letter of Accommodation (LOA) will be available to generate for each course. The LOA must be given to each course instructor by the student and followed up with a discussion. This should be done as early in the semester as possible as accommodations are not retroactive. More information can be found at <u>osas.usc.edu</u>. You may contact OSAS at (213) 740-0776 or via email at <u>osasfrontdesk@usc.edu</u>.

### **Student Financial Aid and Satisfactory Academic Progress:**

To be eligible for certain kinds of financial aid, students are required to maintain Satisfactory Academic Progress (SAP) toward their degree objectives. Visit the <u>Financial Aid Office webpage</u> for <u>undergraduate</u>and <u>graduate-level</u> SAP eligibility requirements and the appeals process.

### **Support Systems:**

### Counseling and Mental Health - (213) 740-9355 – 24/7 on call

Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

### <u>988 Suicide and Crisis Lifeline</u> - 988 for both calls and text messages – 24/7 on call

The 988 Suicide and Crisis Lifeline (formerly known as the National Suicide Prevention Lifeline) provides free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week, across the United States. The Lifeline consists of a national network of over 200 local crisis centers, combining custom local care and resources with national standards and best practices. The new, shorter phone number makes it easier for people to remember and access mental health crisis services (though the previous 1 (800) 273-8255 number will continue to function indefinitely) and represents a continued commitment to those in crisis.

<u>Relationship and Sexual Violence Prevention Services (RSVP)</u> - (213) 740-9355(WELL) – 24/7 on call Free and confidential therapy services, workshops, and training for situations related to gender- and powerbased harm (including sexual assault, intimate partner violence, and stalking).

## Office for Equity, Equal Opportunity, and Title IX (EEO-TIX) - (213) 740-5086

Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants.

### Reporting Incidents of Bias or Harassment - (213) 740-2500

Avenue to report incidents of bias, hate crimes, and microaggressions to the Office for Equity, Equal Opportunity, and Title for appropriate investigation, supportive measures, and response.

## The Office of Student Accessibility Services (OSAS) - (213) 740-0776

OSAS ensures equal access for students with disabilities through providing academic accommodations and auxiliary aids in accordance with federal laws and university policy.

### USC Campus Support and Intervention - (213) 740-0411

Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity, Equity and Inclusion - (213) 740-2101

Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

## USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call

Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

<u>USC Department of Public Safety</u> - UPC: (213) 740-6000, HSC: (323) 442-1200 – 24/7 on call Non-emergency assistance or information.

## Office of the Ombuds - (213) 821-9556 (UPC) / (323-442-0382 (HSC)

A safe and confidential place to share your USC-related issues with a University Ombuds who will work with you to explore options or paths to manage your concern.

## <u>Occupational Therapy Faculty Practice</u> - (323) 442-2850 or <u>otfp@med.usc.edu</u>

Confidential Lifestyle Redesign services for USC students to support health promoting habits and routines that enhance quality of life and academic performance.