UVU UTAH VALLEY UNIVERSITY™

Master Course Syllabus

For additional course information, including prerequisites, corequisites, and course fees, please refer to the Catalog: https://catalog.uvu.edu/

Semester: Spring
Course Prefix: CHEM
Course Title: Physical Chemistry 2

Year: 2025
Course and Section #: 3070-001
Credits: 4

Course Description
Provides an advanced discussion of quantum mechanics, including solutions to the Schrodinger wave equation. Connects quantum mechanics with observables, including spectroscopy.

Course Attributes
This course has the following attributes:
☐ General Education Requirements
☐ Global/Intercultural Graduation Requirements
☐ Writing Enriched Graduation Requirements
☐ Discipline Core Requirements in Program
☒ Elective Core Requirements in Program
☐ Open Elective
Other: *Click here to enter text.*

Instructor Information
Instructor Name: Dr. Matthew Horn

Student Learning Outcomes
1. One objective of this course is to develop student understanding of the following chemical concepts:
    *   Quantum Mechanics
    *   Atomic Structure
    *   Molecular Structure
2. A second objective of this course is to develop student ability to:

    *   Process information in graphical, textual, and mathematical formats
    *   Solve genuine problems using numeric and algebraic conventions
    *   Develop critical thinking skills

Course Materials and Texts
Physical Chemistry: A Molecular Approach by Donald A. McQuarrie and John D. Simon

Course Requirements

Course Assignments, Assessments, and Grading Policy
Written Homework performed in a chapterly fashion 40%
Video Homework performed in a chapterly fashion 15%
Final Presentation performed finally as a presentation 5%
3 Midterms taken in the middle of the term 30%
Comprehensive Final Exam taken finally in a comprehensive fashion 10%

This course will work under a total point system. That is, points for each assignment/test will be summed and compared to the following scale:

Letter Grade	Total Needed	Letter Grade	Total Needed	Letter Grade	Total Needed
A	933 ⅓	B-	800	D+	666 ⅔
A-	900	C+	766 ⅔	D	633 ⅓
B+	866 ⅔	C	733 ⅓	D-	600
B	833 ⅓	C-	700	E	<600

Required or Recommended Reading Assignments
Chapters 1-13 in McQuarrie and Simon

General Description of the Subject Matter of Each Lecture or Discussion
1.1 Objectives for this section include
- Be familiar with black-body radiators
- Apply Stefan-Boltzmann's Law to estimate total light output from a radiator
- Apply Wien's Displacement Law to estimate the peak wavelength (or frequency) of the output from a black body radiator
- Understand the Rayleigh-Jeans Law and how it fails to properly model black-body radiation

1.2 Objectives for this section include
- To understand how energy is quantized in blackbody radiation

1.3 Objectives for this section include
- To be familiar with the photoelectron effect for bulk materials
- Understand how the photoelectron kinetic energy and intensity vary as a function of incident light wavelength
- Understand how the photoelectron kinetic energy and intensity vary as a function of incident light intensity
- Describe what a workfunction is and relate it to ionization energy
- Describe the photoelectric effect with Einstein's quantized photon model of light

1.4 Objectives for this section include
- To introduce the concept of absorption and emission line spectra and describe the Balmer equation to describe the visible lines of atomic hydrogen.

1.5 Objectives for this section include

- Describe Rydberg's theory for the hydrogen spectra.
- Interpret the hydrogen spectrum in terms of the energy states of electrons.

1.6 Objectives for this section include
- To introduce the wave-particle duality of light extends to matter
- To describe how matter (e.g., electrons and protons) can exhibit wavelike properties, e.g., interference and diffraction patterns
- To use algebra to find the de Broglie wavelength or momentum of a particle when either one of these quantities is given

1.7 Objectives for this section include
- To present the experimental evidence behind the wave-particle duality of matter

1.8 Objectives for this section include
- Introduce the fundamentals behind the Bohr Atom and demonstrate it can predict the Rydberg's equation for the atomic spectrum of hydrogen

1.9 Objectives for this section include
- To understand that sometime you cannot know everything about a quantum system as demonstrated by the Heisenberg uncertainly principle.

Chapter 2: waves

2.1 Objectives for this section
- To introduce the wave equation including time and position dependence

2.2 Objectives for this section

- To be introduced to the *Separation of Variables* technique as method to solved wave equations

2.3 Objectives for this section
- Explore the basis of the oscillatory solutions to the wave equation
- Understand the consequences of boundary conditions on the possible solutions
- Rationalize how satisfying boundary conditions forces quantization (i.e., only solutions with specific wavelengths exist)

2.4 Objectives for this section

- Separate the wave equation into individual spatial and temporal problems and solve them.
- Demonstrate that the general solution can be a superposition of solutions (normal modes)

2.5 Objectives for this section include
- To apply the wave equations to a two-dimensional membrane (rectangles and circles)
- To recognize the possible geometries of a nodes in two-dimensional systems

Chapter 3: The particle in a box model

3.1 Objectives for this section include
- To be introduced to the general properties of the Schrödinger equation and its solutions.

3.2 Objectives for this section include
- Classical-Mechanical quantities are represented by linear operators in Quantum Mechanics
- Understand that "algebra" of scalars and functions do not always to operators (specifically the commutative property)

3.3 Objectives for this section include
- To recognize that each quantum mechanical observable is determined by solve by an eigenvalue problem with different operators for different observable
- Confirm if a specific wavefunction is an eigenfunction of a specific operation and extract the corresponding obserable (the eigenvalue)
- To recognize that the Schrödinger equation, just like all measurable, is also an eigenvalue problem with the eigenvalue ascribed to total energy
- Identity and manipulate several common quantum mechanical operators

3.4 Objectives for this section include
- To understand that wavefunctions can have probabilistic interpretations.
- To calculate the probabilities directly from a wavefunctions

3.5 Objectives for this section include
- Solve the particle-in-a-box model used to describing a trapped particle in 1 D well
- Characterize the particle-in-a-box eigenstates (i.e., wavefunctions) and the eigenenergies as a function of the quantum number
- Demonstrate that the eigenstates are orthogonal

3.6 Objectives for this section include
- Calculate the probability of an event from the wavefunction
- Understand the utility and importance of normalizing wavefunctions
- Demonstrate how to normalize an arbitrary wavefunction

3.7 Objectives for this section include
- Calculate the expectation value for a measurement
- Apply the expectation value concept to calculate average properties of a particle in a box model
- Understand the origin of a zero-point energy/zero-point motion.
- Extend the concept of orthogonality from vectors to mathematical functions (and wavefunctions).

3.8 Objectives for this section include
- Expand on the introduction of Heisenberg's Uncertainty Principle by calculating the $\Delta x \Delta x$ or $\Delta p \Delta p$ directly from the wavefunction

3.9 Objectives for this section include
- To demonstrate how the particle in 1-D box problem can extend to a particle in a 3D box
- Introduction to nodal surfaces (e.g., nodal planes)

4.1 Objectives for this section include
- Introduce the first postulate of quantum mechanics
- Recognize invalid wavefunction categories

4.2 Objectives for this section include
- Understand how the correspondence principle argues that a unique quantum operator exists for every classical observable
- .Recognize several of the commonly used quantum operators

4.3 Objectives for this section include
- To be introduced to the role of eigenvalue equations in obtaining observables from a system
- Understand how expectation values are calculated if the wavefunctions is not an eigenstate of the operator for the observable.

4.4 Objectives for this section include
- Recognize the differences between the time-dependent and the time-independent Schrödinger equations
- To distinguish between stationary and non-stationary wavefunctions

4.5 Objectives for this section include
- Understand the properties of a Hermitian operator and their associated eigenstates
- Recognize that all experimental observables are obtained by Hermitian operators

4.6 Objectives for this section include
- To connect the Heisenberg Uncertainty principle to the commutation relations.
- Develop proficiency in calculating the commutator of two operators.

5.1 Objectives for this section include
- To understand the classical harmonic oscillator
- To solve the classical harmonic oscillator

5.2 Objectives for this section include
- To understand the role of reduced mass in the solution to the harmonic oscillator
- To solve the quantum mechanical harmonic oscillator

5.3 Objectives for this section include
- Understand the utility and limits of using the quantum harmonic oscillator as a model for molecular vibrations

5.4 Objectives for this section include
- To understand the quantum number that emerges from the solution to the quantum mechanical harmonic oscillator

5.5 Objectives for this section include
- Understand how the quantum harmonic oscillator model can be used to interpret the infrared spectra of diatomic molecules
- Understand the origin of the transition moment integral and selection rules and how they are related

5.6 Objectives for this section include
- The Equation for a Harmonic-Oscillator Model of a Diatomic Molecule Contains the Reduced Mass of the Molecule

5.7 Objectives for this section include
- Understand key properties of the Hermite polynomials including orthogonality and symmetry.
- Be proficient at using symmetries of integrands to quickly solve integrals.

5.8 Objectives for this section include
- Compare the classical and quantum rigid rotor in three dimensions
- Demonstrate how to use the Separation of Variable technique to solve the 3D rigid rotor Schrödinger Equation
- Identify and interpret the two quantum numbers for a 3D quantum rigid rotor including the range of allowed values
- Describe the wavefunctions of the 3D quantum rigid rotor in terms of nodes, average displacements and most probable displacements
- Describe the energies of the 3D quantum rigid rotor in terms of values and degeneracies

5.9 Objectives for this section include
- Demonstrate how to use the 3D rigid rotor to describe a rotating diatomic molecules
- Demonstrate how microwave spectroscopy can get used to characterize rotating diatomic molecules
- Interpret a simple microwave spectrum for a diatomic molecule

6.1 Objectives for this section include
- Understand that the model of the hydrogen atom can be solved exactly

6.2 Objectives for this section include
- Understand the relationship between the spherical harmonics and the solution to the quantum mechanical hydrogen atom
- Demonstrate how to derive the quantum numbers for the different solutions to the quantum mechanical hydrogen atom

6.3 Objectives for this section include
- Demonstrate that the three components of angular momentum cannot be measured simultaneously with arbitrary precision

6.4 Objectives for this section include
- Demonstrate that the atomic orbitals for the quantum mechanical hydrogen atom depend upon three quantum numbers

6.5 Objectives for this section include
- Demonstrate that s-orbitals are Spherically Symmetric

6.6 Objectives for this section include
- To relate the classical orbital angular momentum for an particle to the quantum equivalent

- Characterize the mangnitude and orientation of orbital angular momentum for an electron in terms of quantum numbers

6.7 Objectives for this section include
- Adding electrons to the quantum hydrogen atom results in analytically unsolvable Schrödinger Equations (they exist, we just do not have analytical forms for them)
- A basic aspect of the corresponding multi-electron Hamiltonians is that they are NOT separable with respect to the spatial coordinate of each electron
- The solutions to multi-electron Schrödinger Equations are called multi-electron wavefunctions and they are often approximated as a product of single-electron wavefunctions (called the orbital approximation).

7.1 Objectives for this section include
- Appreciate the complexity of solving muliti-electron atoms
- Characterize multi-electron interactions within shielding and penetration concepts
- Use the variational method as an approximation to study insolvable problems
- User variational method to evaluate the effective nuclear charge for a specific atom

7.2 Objectives for this section include
- Understand how the variational method can be expanded to include trial wavefunctions that are a linear combination of functions with coefficients that are the parameters to be varied.
- To be able to construct secular equations to solve the minimization procedure intrinsic to the variational method approach.
- To map the secular equations into the secular determinant
- To understand how the Linear Combination of Atomic Orbital (LCAO) approximation is a specific application of the linear variational method.

7.3 Objectives for this section include
- Demonstrate that variational problems can include changing parameters within the elements (normal variational method) and changing coefficients of a basis set (linear variational method)

7.4 Objectives for this section include
- Use perturbation theory to approximate the energies of systems as a series of perturbation of a solved system.
- Use perturbation theory to approximate the wavefunctions of systems as a series of perturbation of a solved system.

8.1 Objectives for this section include
- Demonstrate how solving electron structure problems are less cluttered by switching to atomic units instead of SI units.

8.2 Objectives for this section include
- Demonstrate that both perturbation theory and variational methods can be used to solve the electron structure of the helium atom.

8.3 Objectives for this section include
- Show how the Hartree approximation can be used to solve for the wavefunctions and energies of multi-electron atoms.

- Understand the orbital approach of independent orbitals is an approximation to a mutlti-electron system with the motions of all electrons coupled together.
- Demonstrate how the Self-Consistent Field (SCF) calculation is needed to support the Hartree approximation

8.4 Objectives for this section include
- Understand the forth quantum number for electrons - spin.
- Understand how spin is connected to magnetic properties of the electrons and atoms.
- Understand how to break degeneracy via externally applied magnetic fields in electrons and atoms.

8.5 Objectives for this section include
- Interpret the consequence of exchanging two electrons in a multi-electron atom on the wavelengths
- Connect the Pauli's Exclusion Principle to the permutation symmetry of multi-electron atoms

8.6 Objectives for this section include
- Understand how the Pauli Exclusion principle affects the electronic configuration of multi-electron atoms
- Understand how determinantal wavefunctions (Slater determinants) ensure the proper symmetry to electron permutation required by Pauli Exclusion Principle.
- Connect the electron permutation symmetry requirement to multi-electron wavefunctions to the Aufbau principle taught in general chemistry courses

8.7 Objectives for this section include
- Understand how the Hartree method is expanded to include symmetrized mulit-electron determential wavefunctions via the Hartree-Fock equations.
- Understand how to calculate the orbital energies from HF theory.
- Apply HF theory with Koopman's theory to estimate ionization energies and electron affinities.

8.8 Objectives for this section include
- Understand how electron configurations results in different manifestations of angular momenta (both oribital and spin)
- Describe the manifestations in atoms via atomic term symbols

8.9 Objectives for this section include
- Compare two spin-orbit coupling schemes that couple the total spin angular momenta and total orbital angular momenta of a multi-electron spectra

8.10 Objectives for this section include
- Define Hund's three rules
- Use Hund's three rules to predict the lowest energy configuration and term symbols for multi-electron systems

8.11 Objectives for this section include
- Demonstrate how spin-orbit coupling is experimentally observed in atomic spectra
- Use atomic terms symbols to ascribe transitions to specific angular momenta states described by atomic term symbols

9.1 Objectives for this section include
- Understand the need to introduce an approximation like the Born-Oppenheimer approximation to solve multi-electron systems
- Understand the basis of parameterization involved in using the Born-Oppenheimer approximation

9.2 Objectives for this section include
- Understanding the successful application of the Born-Oppenheimer approximation to the hydrogen molecular ion

9.3 Objectives for this section include
- Understanding the necessity of the overlap integral to determine the molecular orbitals of the hydrogen molecular ion

9.4 Objectives for this section include
- Identify the nature of the energy of molecular orbitals of a diatomic as a function of intermolecular distance
- Identify the three integrals involved in calculation the total Molecular Orbital Energy: coulomb Integral, exchange integral, and overlap integral

9.5 Objectives for this section include
- Characterize the bonding and anti-bonding molecular orbitals in H+

9.6 Objectives for this section include
- Understand the antisymmetric electronic wavefunction coupled with the orbital approximation places both electrons in a bonding orbital in the H_2 molecule

9.7 Objectives for this section include
- Understand how to generate molecular orbitals using the LCAO-MO method

9.8 Objectives for this section include
- Using bond order as a metric for the existence of molecules

9.9 Objectives for this section include
- Understanding the actual mathematical nature of the Pauli Exclusion Principle

9.10 Objectives for this section include
- To describe the connection between bond order, bond length and bond energy in diatomic molecules
- To explain the observed paramagnetic properties of molecular oxygen with Molecular Orbital theory

9.11 Objectives for this section include
- Understanding how photoelectron spectroscopy experimentally confirms molecular orbitals

9.12 Objectives for this section include
- Understand how molecular orbital theory applies to heteronuclear diatomic molecules

9.13 Objectives for this section include
- Understand how SCF-LCAO-MO Wavefunctions are Molecular Orbitals formed from a Linear Combination of Atomic Orbitals and Whose Coefficients Are Determined Self-Consistently

9.14 Objectives for this section include
- Understand how Molecular Term Symbols Describe Electronic States of Molecules

9.15 Objectives for this section include
- Understand how molecular term symbols designate symmetry

9.16 Objectives for this section include
- Understand that most molecules have excited electronic states

10.1 Objectives for this section include
- Introduce hybrid orbital to explain non-linear molecular structure

10.2 Objectives for this section include
- Understand how valence bond theory explains the geometric structure of water

10.3 Objectives for this section include
- Understand how molecular orbital theory shows how structure can vary between similar molecules

10.4 Objectives for this section include
- Demonstrate how photoelectron spectroscopy can be used to resolve the absolute energies of molecular orbitals
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10.5 Objectives for this section include
- Demonstrate how Hückel's theory approximates the full molecular orbital picture of molecules by treating the $\sigma\sigma$-bonding and $\pi\pi$-bonding networks independently.

10.6 Objectives for this section include
- Apply Hückel theory to an extended $\pi\pi$-bonding network
- Identify the origin of delocalization energy from Hückel theory and relate it to resonances structures in valence bond theory

10.7 Objectives for this section include
- Apply Hückel theory to describing the pi bonding in cyclical conjugated system
- Identify the origin of aromaticity within Hückel theory to describe extra stabilization in certain cyclical conjugated systems

Required Course Syllabus Statements

Generative AI
Generative AI exists.

Using Remote Testing Software
☒ This course does not use remote testing software.

☐ This course uses remote testing software. Remote test-takers may choose their remote testing locations. Please note, however, that the testing software used for this may conduct a brief scan of remote test-takers' immediate surroundings, may require use of a webcam while taking an exam, may require the microphone be on while taking an exam, or may require other practices to confirm academic honesty. Test-takers therefore shall have no expectation of privacy in their test-taking location during, or immediately preceding, remote testing. If a student strongly objects to using test-taking software, the student should contact the instructor at the beginning of the semester to determine whether alternative testing arrangements are feasible. Alternatives are not guaranteed.

Required University Syllabus Statements

Accommodations/Students with Disabilities
Students needing accommodations due to a permanent or temporary disability, pregnancy or pregnancy-related conditions may contact UVU Accessibility Services at accessibilityservices@uvu.edu or 801-863-8747.

Accessibility Services is located on the Orem Campus in BA 110.

Deaf/Hard of Hearing students requesting ASL interpreters or transcribers can contact Accessibility Services to set up accommodations. Deaf/Hard of Hearing services can be contacted at DHHservices@uvu.edu

DHH is located on the Orem Campus in BA 112.

Academic Integrity
At Utah Valley University, faculty and students operate in an atmosphere of mutual trust. Maintaining an atmosphere of academic integrity allows for free exchange of ideas and enables all members of the community to achieve their highest potential. Our goal is to foster an intellectual atmosphere that produces scholars of integrity and imaginative thought. In all academic work, the ideas and contributions of others must be appropriately acknowledged and UVU students are expected to produce their own original academic work.

Faculty and students share the responsibility of ensuring the honesty and fairness of the intellectual environment at UVU. Students have a responsibility to promote academic integrity at the university by not participating in or facilitating others' participation in any act of academic dishonesty. As members of the academic community, students must become familiar with their rights and responsibilities. In each course, they are responsible for knowing the requirements and restrictions regarding research and writing, assessments, collaborative work, the use of study aids, the appropriateness of assistance, and other issues. Likewise, instructors are responsible to clearly state expectations and model best practices.

Further information on what constitutes academic dishonesty is detailed in UVU Policy 541: *Student Code of Conduct*.

Equity and Title IX
Utah Valley University does not discriminate on the basis of race, color, religion, national origin, sex, sexual orientation, gender identity, gender expression, age (40 and over), disability, veteran status, pregnancy, childbirth, or pregnancy-related conditions, citizenship, genetic information, or other basis protected by applicable law, including Title IX and 34 C.F.R. Part 106, in employment, treatment, admission, access to educational programs and activities, or other University benefits or services. Inquiries about nondiscrimination at UVU may be directed to the U.S. Department of Education's Office for Civil Rights or UVU's Title IX Coordinator at 801-863-7999 – TitleIX@uvu.edu – 800 W University Pkwy, Orem, 84058, Suite BA 203.

Religious Accommodation
UVU values and acknowledges the array of worldviews, faiths, and religions represented in our student body, and as such provides supportive accommodations for students. Religious belief or conscience broadly includes religious, non-religious, theistic, or non-theistic moral or ethical beliefs as well as participation in religious holidays, observances, or activities. Accommodations may include scheduling or due-date modifications or make-up assignments for missed class work.
To seek a religious accommodation, a student must provide written notice to the instructor and the Director of Accessibility Services at accessibilityservices@uvu.edu. If the accommodation relates to a scheduling conflict, the notice should include the date, time, and brief description of the difficulty posed by the conflict. Such requests should be made as soon as the student is aware of the prospective scheduling conflict.

While religious expression is welcome throughout campus, UVU also has a specially dedicated space for meditation, prayer, reflection, or other forms of religious expression.