Physical Chemistry II

The University of Toledo
Department of Chemistry and Biochemistry
(CHEM 3740, Section 001)

Instructor:	Xiche Hu	**Offered**:	Spring 2022
Email:	xhu@utoledo.edu	**Course Website**:	Blackboard Learn
Office Hours:	MW 2:00 AM - 3:00 PM	**Class Location**:	Bowman Oddy 2059
Office Location:	Wolfe Hall 2277	**Class Day/Time**:	MW 1:00 to 1:55 PM
Instructor Phone:	(419)530-1513	**Credit Hours**:	3

CATALOG/COURSE DESCRIPTION

Fundamental theories and basic laws of chemistry with emphasis on their mathematical development. Structure of matter, statistical and quantum mechanics, reaction dynamics, spectroscopy.

Web site **https://blackboard.utdl.edu**

SPECIAL COURSE EXPECTATIONS DURING COVID-19

Maintaining a safe campus during the ongoing COVID-19 pandemic remains a top priority. UToledo continues to follow the guidance of the U.S. Centers for Disease Control and Prevention and Ohio Department of Health to keep our campus safe.

ATTENDANCE

The University of Toledo has a missed class policy. It is important that students and instructors discuss attendance requirements for the course. Before coming to campus each day, students should take their temperature and complete a self-assessment for symptoms of COVID-19, such as cough, chills, fatigue or shortness of breath. Anyone with a temperature at or above 100.0 degrees Fahrenheit or who is experiencing symptoms consistent with COVID-19 should not come to campus and contact their primary care physician or the University Health Center at 419.530.5549. For more information on the symptoms of COVID-19, please go to https://www.cdc.gov/coronavirus/2019-ncov/symptoms-testing/symptoms.html

COVID-19 testing for sick students is available on both Main Campus and Health Science Campus. Call 419.383.4545 for an appointment. Absences due to COVID-19 quarantine or isolation requirements **are** considered excused absences. Students should notify their instructors and follow the protocols summarized in this document on Navigating COVID-Related Course Concerns.

In the event that you have tested positive for COVID-19 or have been diagnosed as a probable case, please review the CDC guidance on self-isolation and symptom monitoring, and report the disclosure to the Division of Student Affairs by emailing StudentAffairs@utoledo.edu or by connecting with their on-call representative at 419.343.9946. Disclosure is voluntary and will only be shared on a need to know basis with staff such as in the Office of Student Advocacy and Support, The Office of Residence Life, and/or the Office of Accessibility and Disability Resources to coordinate supportive measures and meet contact tracing requirements.

FACE COVERINGS
Face coverings are required while on campus, except while eating, alone in an enclosed space, or outdoors practicing social distancing. Students will not be permitted in class without a face covering. If you have a medical reason preventing you from wearing a face covering due to a health condition deemed high-risk by the CDC, submit an online application to request an accommodation through the Office of Accessibility and Disability Resources. Students will need to provide documentation that verifies their health condition or disability and supports the need for accommodations. Students already affiliated with the Office of Accessibility and Disability Resources who would like to request additional accommodations due to the impact of COVID-19, should contact their accessibility specialist to discuss their specific needs. You may connect with the office by calling 419.530.4981 or sending an email to StudentDisability@utoledo.edu.

VACCINATION
Doctors and other health care professionals agree that the best way to protect ourselves and each other is to get vaccinated. Case data clearly show that vaccines remain highly effective at preventing serious illness from COVID, including the highly contagious delta variant. If you have not yet received your COVID vaccine, the University encourages you do so as soon as possible. No appointment is needed to get the shot at the UTMC Outpatient Pharmacy, University Health Clinic or Main Campus Pharmacy. Once you receive the COVID vaccination, please register on the COVID Vaccine Registry site at: https://utvaccinereg.utoledo.edu/.

SPECIAL NOTES
It's important to note, that based on the unpredictability of the COVID-19 virus, things can change at any time. So please be patient and understanding as we move through the semester. I also ask that you keep me informed of concerns you may have about class, completing course work/assignments timely and/or health concerns related to COVID.

Course Objectives:

This course covers the fundamental principles of quantum theory and their application to the atomic and molecular systems of interest to chemists in the general area of molecular structure, atomic and molecular spectroscopy, statistical thermodynamics, and chemical reaction dynamics.

Course Organization

Three lectures will be given each week. At the start of each class period reading will be assigned for the following period. You will be expected to have read the chapter prior to coming to class. You should review the lecture notes as soon as possible after class and also before the next lecture. You are encouraged to ask questions during the lecture. Only a questioning mind can learn.

Homework

Physical chemistry is a demanding subject due both to its exceptional breadth and to its rigor. Mechanically, it can be hard to calculate the correct answer because of algebra complexities or unit conversions. Conceptually, you will have to find the right technique to solve a problem or identify the formula appropriate for the problem. There are no shortcuts. To learn physical chemistry, you must practice problem-solving. The assigned homework problems will represent material that is essential for you to understand in order to do well on the exams, and in the course. Homework problems will be assigned during the semester. There will be a total of 12 problem sets. Each set will usually be due one week after it is assigned. Late assignments will not be accepted. Problem sets will be collected and solutions will be posted on the course website after the assignment is due. You are encouraged to discuss the problems among yourselves as well as with the instructor.

Exams and Course Grades

There will be six short quizzes, three midterm exams given during regular class periods (scheduled tentatively on Feb. 18, March 25 and April 24) and a cumulative final exam on May 6. The quizzes will cover material from the preceding chapter; each will count 20 points. At the end of the semester your lowest quiz score will be dropped, so the total scores from quizzes will be 100 points. Grades will be based on problem sets (only best 10 out of 12 problem sets will be counted), quizzes, and exams weighted as follows:

Item	Points
10 problem sets @ 5 points*	50
5 Quizzes @ 20 points	100
Exam 1	100
Exam 2	100
Exam 3	100
Final Exam	200
Total points	**650**

Note: * Homework is mandatory. NO grade will be given without clear evidence of a serious effort on completing all homework assignments.

Letter grades will be assigned based on your total percentage scores, taking into consideration of the degree of difficulty of exams. As a guideline, it is expected that the distribution of grades will be similar to previous semesters with approximately the following distribution: 20% A, 35% B, 35% C and 10% D. A grade of F may be assigned for very low scores. "+" and "-" grades will be assigned to adequately reflect border-line scores.

All students are required to complete every examination. No makeup examinations will be given. Students who know that they will not be able to take an exam at the scheduled time due to an unresolvable conflict with a major responsibility must provide written documentation to verify the conflicts one week in advance. Students who do not take an exam due to illness, car accident or similar extreme circumstance should inform the instructor in a timely fashion. In all cases of missed examinations, students must complete an Absence Report Form that can be obtained from the Chemistry Department Secretary in the Chemistry Office, Room BO2022. Documentation supporting your excuse must be attached to the form.

Attendance

All students are expected to attend classes. Attendance will be taken during the semester on several randomly selected dates. The frequency of taking attendance can be increased if needed.

To Do Well in This Class

1. Read assignments before lecture. The lectures will be hard (to impossible) to understand without this background.
2. Attend class regularly; do not fall behind.
3. Do the problems! You cannot learn by reading or copying the problem solutions.
4. If you are unable to do a problem, seek help immediately. Peer study groups are an excellent way to get this help, or you can find your instructor.
5. Study the examples in the text and the assigned homework carefully. Most problems and exam questions will be like the examples in the text or problems.
6. Keep track of units. Coming up with a strange unit is a sure sign that something has gone terribly wrong.

Recommended Reference Books

1. Physical Chemistry 4th Ed., by Laidler, Meiser and Sanctuary
2. **Physical Chemistry 7th Ed., by Atkins**
3. **Quantum Chemistry 5th Ed., by Levine**
4. Quantum Chemistry, 2nd Ed, by Lowe
5. Statistical Thermodynamics, by McQuarrie

UNIVERSITY POLICIES

Institutional Classroom Attendance Policy

Please be aware that the university has implemented an attendance policy, which requires faculty to verify student participation in every class a student is registered at the start of each new semester/course. For this course, if you have not attended/participated in class (completed any course activities or assignments) within the first 14 days, I am required by federal law to report you as not attended. Unfortunately, not attending/participating in class impacts your eligibility to receive financial aid, so it is VERY important that you attend class and complete course work in these first two weeks. Please contact me as soon as possible to discuss options and/or possible accommodations if you have any difficulty completing assignments within the first two weeks.

Policy Statement on Non-Discrimination on the Basis of Disability (ADA)

The University is an equal opportunity educational institution. Please read The University's Policy Statement on Nondiscrimination on the Basis of Disability Americans with Disability Act Compliance. Students can find this policy along with other university policies listed by audience on the University Policy webpage (http://www.utoledo.edu/policies/audience.html/#students).

Academic Accommodations

The University of Toledo embraces the inclusion of students with disabilities. We are committed to ensuring equal opportunity and seamless access for full participation in all courses. For students who have an Accommodations Memo from the Office of Accessibility and Disability Resources, I invite you to correspond with me as soon as possible so that we can communicate confidentially about implementing accommodations in this course.

For students who have not established accommodations with the Office of Accessibility and Disability Resources and are experiencing disability access barriers or are interested in a referral to health care resources for a potential disability, please connect with the office by calling 419.530.4981 or sending an email to StudentDisability@utoledo.edu.

ACADEMIC AND SUPPORT SERVICES

Please follow this link to view a comprehensive list of Student Academic and Support Services (http://www.utoledo.edu/studentaffairs/departments.html) available to you as a student.

SAFETY AND HEALTH SERVICES FOR UT STUDENTS

Please use the following link to view a comprehensive list Campus Health and Safety Services available to you as a student.

INCLUSIVE CLASSROOM STATEMENT

In this class, we will work together to develop a learning community that is inclusive and respectful. Our diversity may be reflected by differences in race, culture, age, religion, sexual orientation, gender identity/expression, socioeconomic background, and a myriad of other social identities and life experiences. We will encourage and appreciate expressions of different ideas, opinions, and beliefs so that conversations and interactions that could potentially be divisive turn, instead, into opportunities for intellectual and personal development.

Schedule

Date	Topic	Ch.	Activity
Jan. 19	Introduction		
Jan. 21, 24	**Dawn of the Quantum Era** Observations that didn't fit classical theories 1. Photoelectric effect 2. Blackbody radiation 3. Hydrogen atomic spectrum Wave-Particle Duality 6. Energy of light waves "quantized" (Planck, Einstein) 7. DeBroglie Wave: Particles have wavelike properties 8. Davisson-Germer experiment (Davisson-Germer-Thompson) • Heisenberg uncertainty principle	1	**HW-1**
Jan. 26, 28	**Complex Numbers** **The Classical Wave Equation** 2-1. The One-Dimensional Wave Equation for Motion of a Vibrating String 2-2. The Wave Equation Can Be Solved by the Method of Separation of Variables 2-3. Some Differential Equations Have Oscillatory Solutions 2-4. The General Solution to the Wave Equation Is a Superposition of Normal Modes	2	**QUIZ (1)** **HW-2**
Jan. 31 Feb. 2, 4	**The Schrodinger Equation and Particle-In-A-Box** 3-1. The Schrodinger Equation 3-2. Classical-Mechanical Quantities: Linear Operators in Quantum Mechanics 3-3. The Schrodinger Equation Can be Formulated as an Eigenvalue Problem 3-4. Wave Functions Have a Probabilistic Interpretation 3-5. The Energy of a Particle in a Box Is Quantized 3-6. Wave Functions Must Be Normalized 3-7. The Average Momentum of a Particle in a Box is Zero 3-8. The Uncertainty Principle 3-9. Particle in a Three-Dimensional Box	3	**QUIZ (2)** **HW-3**
Feb. 7, 9, 11	**Postulates and General Principles of Quantum Mechanics** 4-1. The State of a System Is Completely Specified by its Wave Function 4-2. Quantum-Mechanical Operators Represent Classical-Mechanical Variables 4-3. Observable Quantities Must Be Eigenvalues of Quantum Mechanical Operators 4-4. Time-Dependent Schrodinger Equation 4-5. The Eigenfunctions of Quantum Mechanical Operators Are Orthogonal 4-6. The Physical Quantities Corresponding to Operators That Commute	4	**QUIZ (3)** **HW-4**
Feb. 14, 16, 18, 21	**Harmonic Oscillator and Rigid Rotor: Two Spectroscopic Models** 5-1. A Harmonic Oscillator Obeys Hooke's Law 5-2. The Equation for a Harmonic-Oscillator Model of a Diatomic Molecule 5-3. The Harmonic-Oscillator Approximation for an Internuclear Potential 5-4. The Energy Levels of a Quantum-Mechanical Harmonic Oscillator 5-5. The Harmonic Oscillator Accounts for the IR Spectrum of a Diatomic Molecule 5-6. The Harmonic-Oscillator Wave Functions Involve Hermite Polynomials 5-7. Hermite Polynomials Are Either Even or Odd Functions 5-8. The Energy Levels of a Rigid Rotator 5-9. The Rigid Rotator Is a Model for a Rotating Diatomic Molecule	5	**QUIZ** **(1-4)** **HW-5**
Feb. 23	**Midterm EXAM #1: Chaps. 1 to 5**		
Feb. 25, 28, March 2, 4	**Hydrogen Atom and Atomic Orbitals** 6-1. The Schrodinger Equation for the Hydrogen Atom Can Be Solved Exactly 6-2. The Wave Functions of a Rigid Rotator Are Called Spherical Harmonics 6-3. Components of Angular Momentum 6-4. Hydrogen Atomic Orbitals Depend upon Three Quantum Numbers	6	**HW-6**

	6-5. s Orbitals Are Spherically Symmetric 6-6. Three p Orbitals, Five d Orbitals 6-7. The Schrodinger Equation for the Helium Atom Cannot Be Solved Exactly		
March 7 -11:	**Spring Break**		
March 14, 16	**Multielectron Atoms** 8-1. Atomic and Molecular Calculations Are Expressed in Atomic Units 8-2. Pertubation Theory and the Variational Method for Helium 8-3. Hartree-Fock Equations Are Solved by the Self-Consistent Field Method 8-4. An Electron Has An Intrinsic Spin Angular Momentum 8-5. Wave Functions Must Be Antisymmetric 8-6. Antisymmetric Wave Functions Can Be Represented by Slater Determinants 8-7. Hartree-Fock Calculations Give Good Agreement with Experimental Data	8	**QUIZ (6) HW-7**
March 18, 21, 23	**Bonding in molecules** 6. The Born-Oppenheimer Approximation 7. Diatomic molecules 8. Polyatomic molecules	9, 10	**HW-8**
March 25	**Midterm Exam #2: Chaps. 6, 8, 9, 10**		
March 28, 30	**Symmetry: Group Theory**	12	**HW-9**
April 1, 4 6, 8, 11	**Molecular Spectroscopy** 13-1. Regions of the Electromagnetic Spectrum: Different Molecular Processes 13-2. Rotational Transitions Accompany Vibrational Transitions 13-3. Unequal Spacing of the Lines in a Vibration-Rotation Spectrum 13-4. The Lines in a Pure Rotational Spectrum Are Not Equally Spaced 13-5. Overtones Are Observed in Vibrational Spectra 13-6. Electronic Spectra Contain Electronic, Vibrational, and Rotational Information 13-7. The Franck-Condon Principle 13-11. Selection Rules Are Derived from Time-Dependent Perturbation Theory 13-12. The Selection Rule in the Rigid Rotator Approximation 13-13. The Harmonic-Oscillator Selection Rule	13	**HW-10**
April 13, 15, 18, 20	**Statistical Mechanics** • Averaging and Probability Distributions • The Boltzmann Factor And Partition Functions • The Partition Function of a System of Independent, Distinguishable Particles • The Partition Function of a System of Independent, Indistinguishable Particles • Effect of Quantum Size on the Population of States • Internal Energy and the Partition Function • Entropy and the Partition Function • Other Thermodynamic Functions from Partition Functions • Equilibrium Constants and Statistical Mechanics	17, 18	**HW-11**
April 22	**Review**		**Quiz (17-18)**
April 25,	**Midterm Exam #3: Chaps. 12, 13, 17, 18**		
April 27	**Transitional State Theory** • Potential Energy Surfaces • Reaction Coordinate • Transitional State Theory	30	
April 29	**Review for the Final Exam**		
May 6	**Final Exam: Cumulative** (12:30 to 2:30 PM)		