

CHEM 5350 Quantum Mechanics

The University of Texas at Tyler, Spring 2024

Class Meeting Information

MoWeFr 9:05AM - 10:00AM
Ratliff Building North (RBN) 03041
01/16/2024 - 05/04/2024

Instructor Information

Prof. Kai Zhang
Office: RBS 3007A
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Office Hours: MWF: 10:10am – 12:00am and open-door policy

Description

A rigorous study of the fundamental principles of quantum mechanics as it applies to molecular structure, dynamics, and spectroscopy. Quantum theory is applied to some simple systems followed by a description of approximation methods that are used to solve real chemical problems. An overview of modern computational methods will also be described.

Prerequisite: CHEM 3354 or equivalent.

Learning Objectives

By the end of the course the students should be able to

- Understand the general principles of quantum mechanics on a rigorous basis
- Solve Schrödinger equation for simple systems
- Apply approximation methods to calculate structures of atoms and molecules
- Articulate the concepts that set the foundation of computational chemistry

Required Textbook(s)

None

Other References and Reading Materials

- *Quantum Chemistry An Introduction* by Walter Kauzmann
- *Mathematics for Quantum Chemistry* by Jay Martin Anderson
- *Quantum Mechanics in Chemistry* by Melvin W. Hanna
- *Elementary Quantum Chemistry* by Frank L. Pilar
- *Atoms and Molecules: An Introduction for Students of Physical Chemistry* by Martin Karplus and Richard N. Porter
- *Introduction to Quantum Mechanics with Applications to Chemistry* by Linus Pauling and E. Bright Wilson, Jr.
- *Quantum Chemistry* by Ira N. Levine

- *Quantum Mechanics for Chemistry* by Seogjoo J. Jang
<https://link.springer.com/book/10.1007/978-3-031-30218-3>

Evaluation and Grade

Course work	%
Homework(x10)	5% x 10 = 50%
Quiz(x3)	5% x 3 = 15%
Final Exam	35%

The total number of points you attained on all graded work determines your final grade.

Grade	%
A	90 - 100
B	80 - 89
C	70 - 79
D	60 - 69
F	below 59

Topic Schedule (tentative)

Timeframe	Topic
Review of Mathematics and Physics	
Week 1	Linear Algebra and Vector Calculus
Week 2	Orthogonal Functions and Differential Equations
Week 3	Classical Mechanics and Early Quantum Theory
General Formalism of Quantum Mechanics	
Week 4	Schrödinger Equation and Translational Motion
Week 5	General Principles of Quantum Mechanics
Week 6	Vibration and Harmonic Oscillator
Week 7	Angular Momentum and Rigid Rotator
Week 8	Dirac Notation and Hilbert Space
Week 9	Approximation Methods: Variation and Perturbation
Atomic Structure	
Week 10	Hydrogen-like Atom/Ions
Week 11	Electron Spin and Identical Particles
Week 12	Hartree-Fock Self-Consistent Field (SCF) Method for Multi-electron Atoms
Molecular Structure	
Week 13	Hydrogen Molecule Ion and Hydrogen Molecule
Week 14	Hartree-Fock Self-Consistent Field (SCF) Method for Molecules

University Resources for Students
Resources to assist you in this course

- [UT Tyler Student Accessibility and Resource \(SAR\) Office](#)[Links to an external site.](#) (provides needed accommodations to students with document needs related to access and learning)
- [UT Tyler Writing Center](#)[Links to an external site.](#)
- [The Mathematics Learning Center](#)[Links to an external site.](#)
- [UT Tyler PASS Tutoring Center](#)[Links to an external site.](#)
- [UT Tyler Supplemental Instruction](#)[Links to an external site.](#)
- [Upswing \(24/7 online tutoring\) - covers nearly all undergraduate course areas](#)[Links to an external site.](#)[Links to an external site.](#)
- [Robert Muntz Library](#)[Links to an external site.](#) and [Library Liaison](#)[Links to an external site.](#)
- [Canvas 101](#)[Links to an external site.](#) (learn to use Canvas, proctoring, Unicheck, and other software)
- LIB 422 -- Computer Lab where students can take a proctored exam
- [The Career Success Center](#)[Links to an external site.](#)
- [UT Tyler Testing Center](#)[Links to an external site.](#)
- [Office of Research & Scholarship Design and Data Analysis Lab](#)[Links to an external site.](#)

Resources available to UT Tyler Students

- [UT Tyler Counseling Center](#) [Links to an external site.](#) (available to all students)
- [My SSP App](#)[Links to an external site.](#) (24/7 access to Student Support Program counseling through phone or chat and online wellness resources available in a variety of languages)
- [Student Assistance and Advocacy Center](#)[Links to an external site.](#)
- [Military and Veterans Success Center](#) [Links to an external site.](#) (supports for all of our military-affiliated students)
- [UT Tyler Patriot Food Pantry](#)[Links to an external site.](#)
- [UT Tyler Financial Aid and Scholarships](#)[Links to an external site.](#)
- [UT Tyler Registrar's Office](#)[Links to an external site.](#)
- [Office of International Programs](#)[Links to an external site.](#)
- [Title IX Reporting](#)[Links to an external site.](#)
- [Patriots Engage](#)[Links to an external site.](#) (available to all students. Get engaged at UT Tyler.)

University Policies and Information

Withdrawing from Class

Students, you are allowed to [withdraw](#) (drop) from this course through the [Withdrawal Portal](#). Withdrawing from classes can impact Financial Aid, Scholarships, Veteran Benefits, Exemptions, Waivers, International Student Status, housing, and degree progress. Please read this page, speak with your instructors, consider your options, and speak with your instructor. UT Tyler faculty and staff are here for our students and often can provide additional support options or student assistance. Please read the implications for withdrawing from a course and the

instructions on using the Withdrawal portal on the [Registrar's Withdrawal page](#). Texas law prohibits students who began college for the first time in Fall 2007 or thereafter from dropping more than six courses during their entire undergraduate career. This includes courses dropped at other 2-year or 4-year Texas public colleges and universities. Consider the impact withdrawing from this class has on your academic progress and other areas, such as financial implications. We encourage you to consult your advisor(s) and financial aid for additional guidance. CAUTION #1: Withdrawing before census day does not mean you get a full refund. Please see the [Tuition and Fee Refund Schedule](#). CAUTION #2: All international students must check with the [Office of International Programs](#) before withdrawing. All international students are required to enroll full-time for fall and spring terms. CAUTION #3: All UT Tyler Athletes must check with the Athletic Academic Coordinator before withdrawing from a course. CAUTION #4: All veterans or military-affiliated students should consult with the [Military and Veterans Success Center](#).

Final Exam Policy

Final examinations are administered as scheduled. If unusual circumstances require that special arrangements be made for an individual student or class, the Dean of the appropriate college, after consultation with the faculty member involved, may authorize an exception to the schedule. Faculty members must maintain student final examination papers for a minimum of three months following the examination date.

Incomplete Grade Policy

If a student, because of extenuating circumstances, is unable to complete all of the requirements for a course by the end of the semester, then the instructor may recommend an Incomplete (I) for the course. The "I" may be assigned in place of a grade only when all of the following conditions are met: (a) the student has been making satisfactory progress in the course; (b) the student is unable to complete all coursework or final exam due to unusual circumstances that are beyond personal control and are acceptable to the instructor, and (c) the student presents these reasons before the time that the final grade roster is due. The semester credit hours for an Incomplete will not be used to calculate the grade point average. The student and the instructor must submit an Incomplete Form detailing the work required and the time by which the work must be completed to their respective department chair or college dean for approval. The time limit established must not exceed one year. Should the student fail to meet all of the work for the course within the time limit, then the instructor may assign zeros to the unfinished work, compute the course average for the student, and assign the appropriate grade. If a grade has yet to be assigned within one year, then the Incomplete will be changed to an F, or NC. If the course was initially taken under the CR/NC grading basis, this may adversely affect the student's academic standing.

Grade Appeal Policy

Disputes regarding grades must be initiated within sixty (60) days from the date of receiving the final course grade by filing a Grade Appeal Form with the instructor who assigned the grade; this is separate from the Application for Appeal form submitted to the Student Appeals Committee, which does not rule on grade disputes as described in this policy. If the student is not satisfied with the decision, the student may appeal in writing to the Chairperson of the

department from which the grade was issued. In situations where there is an allegation of capricious grading, discrimination, or unlawful actions, appeals may go beyond the Chairperson to the Dean of the college from which the grade was issued, with that decision being final. The Grade Appeal form is found in the [Registrar's Form Library](#).

Disability/Accessibility Services

In accordance with Section 504 of the Rehabilitation Act, Americans with Disabilities Act (ADA) and the ADA Amendments Act (ADAAA), the University of Texas at Tyler offers accommodations to students with learning, physical, and/or psychological disabilities. If you have a disability, including a non-visible diagnosis such as a learning disorder, chronic illness, TBI, PTSD, ADHD, or a history of modifications or accommodations in a previous educational environment, you are encouraged to visit <https://hood.accessiblelearning.com/UTTyler> and fill out the New Student application. The Student Accessibility and Resources (SAR) office will contact you when your application has been submitted and an appointment with the Assistant Director Student Accessibility and Resources/ADA Coordinator. For more information, including filling out an application for services, please visit the SAR webpage at <https://www.uttyler.edu/disability-services>, the SAR office located in the University Center, # 3150, or call 903.566.7079."

Military Affiliated Students

UT Tyler honors the service and sacrifices of our military-affiliated students. If you are a student who is a veteran, on active duty, in the reserves or National Guard, or a military spouse or dependent, please stay in contact with your faculty member if any aspect of your present or prior service or family situation makes it difficult for you to fulfill the requirements of a course or creates disruption in your academic progress. It is important to make your faculty member aware of any complications as far in advance as possible. Your faculty member is willing to work with you and, if needed, put you in contact with university staff who are trained to assist you. The [Military and Veterans Success Center \(MVSC\)](#) has campus resources for military-affiliated students. The MVSC can be reached at MVSC@uttyler.edu or via phone at 903.565.5972.

Students on an F-1 Visa

To remain in compliance with Federal Regulations requirements you must do the following:

- Traditional face-to-face classes: Attend classes on the regular meeting days/times.
- Hybrid Classes: Attend all face-to-face classes convened by the instructor and meet with the Office of International Programs according to the schedule set for your specific course.
- Online course: Only one online course can count toward your full-time enrollment. Students are expected to be fully engaged and meet all requirements for the online course.

Academic Honesty and Academic Misconduct

The UT Tyler community comes together to pledge that "Honor and integrity will not allow me to lie, cheat, or steal, nor to accept the actions of those who do." Therefore, we enforce

the [Student Conduct and Discipline policy](#) in the Student Manual Of Operating Procedures (Section 8).

FERPA

UT Tyler follows the Family Educational Rights and Privacy Act (FERPA) as noted in [University Policy 5.2.3](#). The course instructor will follow all requirements to protect your confidential information.

Absence for Official University Events or Activities

This course follows the practices related to approved absences as noted by the Student Manual of Operating Procedures ([Sec. 1 -501](#)).

Absence for Religious Holidays

This course follows the practices related to [Excused Absences for Religious Holy Days as noted in the Catalog](#).

Campus Carry

We respect the right and privacy of students who are duly licensed to carry concealed weapons in this class. License holders are expected to behave responsibly and keep a handgun secure and concealed. More information is available at <http://www.uttyler.edu/about/campus-carry/index.php>.