PHYSICAL CHEMISTRY II

CHEM 3620

Spring 2023

Instructor: Matthew Rowley Office Hours: Daily 10:00 am – 11:00 am

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Please include the course number in the subject line of all correspondence.

Course Description

This course will provide an introduction to quantum mechanics, a topic that is the foundation of all chemistry. During the turn of the 20th century many scientists believed that all of the major questions about science had already been answered and all that was needed was a little refinement. However, led by the experimental discoveries and theoretical models of Einstein, Planck, de Broglie, and others, the scientific world was turned upside down and the miniature physical world of quantum mechanics was discovered. This course will focus on quantum mechanics; full understanding of this topic will require proficient math skills. Therefore, it is highly recommended that students review the math chapters in the text.

Prerequisites: A minimum grade of C (2.0 or above) in CHEM 1220/1225 and Math 1220, and admission to the Chemistry program.

Concurrent requisite: CHEM 3625 – Physical Chemistry Lab II

Course Materials:

- *Physical Chemistry: Thermodynamics, Structure, and Change* by Atkins, de Paula, and Keeler 11th edition (required) ISBN: 978-0-19-876986-6
 - o Applied Mathematics for Physical Chemistry by James R. Barrante (suggested)

—or—

• Mathematics for Physical Chemistry by Robert G. Mortimer (suggested)

Student Learning Outcomes:

- · Students will successfully identify and understand the experiments that led to the discovery of quantum mechanics.
- $\cdot\,$ Students will understand and utilize the fundamental quantum mechanical Schrödinger equation.

- · Students will generate and apply the following mathematical models to real systems:
 - Particle in a Box
 - Harmonic Oscillator
 - Rigid Rotor
- Students will understand how the quantum mechanical models can be used in spectroscopy to predict various structural and chemical properties.
- Students will learn about group theory and how combining it with quantum mechanics provides a powerful tool for understanding the consequences of molecular symmetry (atomic orbital contributions to molecular orbitals, the origin of selection rules, identify the normal modes of vibration for molecules, and determine IR/Raman activity.

Tentative Schedule

This class will meet on Mondays, Wednesdays, and Fridays from 12:00 pm to 12:50 pm in room 128 of the Science Center (SC).

For the best lecture experience, read the indicated textbook chapter *before* each lecture.

	Date	Topic	Chapter
Week 1	M, Jan. 9	The Origins of Quantum Mechanics	7A
	W, Jan. 11	Wavefunctions	7B
	F, Jan. 13	Operators and Observables	7C
Week 2	M, Jan. 16	Martin Luther King Day – No Class!	
	W, Jan. 18	Experiments and Interpretations in QM	**
	F, Jan. 20	Translational Motion	7D
Week 3	M, Jan. 23	Vibrational Motion	7E
	W, Jan. 25	Rotational Motion	7F
	F, Jan. 27	Hydrogenic Atoms	8A
Week 4	M, Jan. 30	Many Electron Atoms	8B
	W, Feb. 1	Atomic Spectra	8C
	F, Feb. 3	Valence-Bond Theory	9A

	Date	Topic	Chapter
Week 5 M, Feb. 6		MO Theory: the Hydrogen Molecule-Ion	9B
	W, Feb. 8	MO Theory: Homonuclear Diatomic Molecules	9C
	F, Feb. 10	MO Theory: Heteronuclear Diatomic Molecules	9D
Week 6	M, Feb. 13	MO Theory: Polyatomic Molecules	9E
	W, Feb. 15	Shape and Symmetry	10A
	F, Feb. 17	Group Theory	юВ
Week 7	M, Feb. 20	President's Day – No Class!	
	W, Feb. 22	Applications of Symmetry	10C
	F, Feb. 24	General Features of Molecular Spectroscopy	11A
Week 8	M, Feb. 27	Spring Break – No Class!	
	W, Mar. 1	Spring Break – No Class!	
	F, Mar. 3	Spring Break – No Class!	
Week 9	M, Mar. 6	Rotational Spectroscopy	11B
	W, Mar. 8	Vibrational Spectroscopy of Diatomic Molecules	11C
	F, Mar. 10	Vibrational Spectroscopy of Polyatomic Molecules	11D
Week 10	M, Mar. 13	Electronic Spectra	11F
	W, Mar. 15	Decay of Excited States	11G
	F, Mar. 17	Lasers and Spectroscopy Special Topics	**
Week 11	M, Mar. 20	General Principles of NMR	12A
	W, Mar. 22	Features of NMR Spectra	12B
	F, Mar. 24	Pulse Technique in NMR	12C
Week 12	M, Mar. 27	Electron Paramagnetic Resonance	12D
	W, Mar. 29	The Boltzmann Distribution	13A
	F, Mar. 31	Molecular Partition Functions	13B

	Date	Topic	Chapter
Week 13	M, Apr. 3	Molecular Energies	13C
	W, Apr. 5	The Canonical Ensemble	13D
	F, Apr. 7	Internal Energy and Entropy	13E
Week 14	M, Apr. 10	Derived Functions	13F
	W, Apr. 12	Electric Properties of Molecules	14A
	F, Apr. 14	Interactions Between Molecules	14B
Week 15	M, Apr. 17	Liquids	14C
	W, Apr. 19	Macromolecules and Self-Assembly	14D-E
	F, Apr. 21	Catch-up/Review Day	
Finals Week	T, Apr. 25	Final Exam — 11:00 – 12:50 Bring a pencil	and scantron

Course Policies and Grading

Grades will be based on the following items:

4 Midterm Exams 40%

Final Exam 15%

Quizzes 15%

Homework 30%

Final Grades will be assigned according to the following grade scale:

Percentage	Grade	Percentage	Grade
100-93.0	A	77.0-73.0	С
93.0-90.0	A-	73.0-70.0	C-
90.0-87.0	B+	70.0–67.0	D+
87.0-83.0	В	67.0-63.0	D
83.0-80.0	B-	63.0-60.0	D-
80.0-77.0	C+	< 60.0	F

Midterm Exams: There are four midterm exams, to be completed in the testing center unless prior arrangements have been made. It is departmental policy that exams not be returned, although students may examine their completed exam and the answer key in my office. Scantron sheets are not required for midterms.

Final Exam: The final exam is comprehensive. The final is produced by the American Chemical Society, and the instructor will not have access to the exam prior to its administration. Therefore, it is to your advantage to learn as much as possible throughout the semester. The test is multiple choice and a scantron will be required.

Homework: The homework assignments will be a combination of problems from the textbook as well as problems that I have written or gathered from various other resources. These assignments are designed to be somewhat challenging and will require diligence in order to complete. They sometimes push the students to think *beyond* the lecture material.

Quizzes: Quizzes will be shorter and more frequent assignments than the regular homework. The difficulty and scope of the questions on quizzes will more closely match what you will see on the exams.

Attendance Policy: Students are expected to attend class. If you must miss class, contact the instructor.

Make-up Work Policy: In general, there will be no opportunity to make up missed work. If you must miss class, please do any assigned work in advance, and arrange to turn it in early.

Miscellany

Important syllabus statements related to ATTENDANCE and COVID-19:

- Q: If a student does NOT want to attend face-to-face this fall, is there another option?
- A: All students who would normally attend face to face classes should plan to do so, unless they are ill or are concerned for their health. However, if a student is ill or concerned for their health, students will be able to complete classes this fall whether they stay home or are here in Cedar City. Digital recording equipment will be installed in each instructional space (classrooms, labs and other venues) so that students can log in and attend face-to-face classes remotely. This will allow any SUU community member to engage in classroom activities in the way they feel comfortable. Faculty will also be able to teach remotely in accordance with their personal health needs. Faculty will likely post the link for how to listen/watch live in the syllabus (and/or Canvas) or simply email it to their students. We recommend to students that they reach out to their faculty to notify them how they will be 'attending' class.

- Q: Would it be possible to participate in courses remotely for the entire fall 2020 semester if desired?
- A: Yes. The intent is that this semester is normal and that students attend face to face classes, however, if they are symptomatic or concerned for their health, they can participate remotely. All students will be able to complete the fall semester from another location. Students should notify their faculty if they are completing the course from a distance rather than attending class in-person. International students will need to be mindful of how this will impact their non-immigrant status and to contact International Affairs if there are any questions.
- **Q:** Do students need special documentation to be allowed to attend classes remotely?
- A: No, students do not need special documentation to attend classes remotely. However, students should notify their faculty if they are completing the course from a distance rather than attending class in-person so expectations can be clearly understood. Remote attendance should be for those who are ill or symptomatic.

ZOOM ETIQUETTE: Your class may utilize the Zoom online conference system. To participate in Zoom meetings, you will need to have a webcam/microphone or a smartphone with the Zoom app. We will adopt the same rules and norms as in a physical classroom (take notes; participate by asking and answering questions; wear classroom-ready clothing). For everyone's benefit:

- · Join the course in a quiet, distraction free location
- · Be aware of your background
- Turn on your video (you may close it after attendance is taken if your internet connection cannot handle having both audio and video going)
- · Mute your microphone unless you are speaking
- · Close browser tabs and software not required for participating in class
- · Remember that our classes are in the Mountain Time zone

The success of this class will depend on the same commitment to learning we all typically bring to the physical classroom.

Scientific Calculator: There are many different ways to calculate figures during homework. It is tempting to rely on Online resources such as http://www.wolframalpha.com, or to simply use a calculator application on a smart phone. During exams, however, any devices capable of connecting to the Internet will *not* be allowed. You will instead need a scientific calculator capable of performing exponentiation and logarithms for the exams. Using this calculator exclusively while doing homework will ensure that you are familiar with it for use during exams.

Academic Integrity: Scholastic dishonesty will not be tolerated and will be prosecuted to the fullest extent (see SUU Policy 6.33). You are expected to have read and understood the current SUU student conduct code (SUU Policy 11.2) regarding student responsibilities and rights, the intellectual property policy (SUU Policy 5.52), information about procedures, and what constitutes acceptable behavior.

Mental Health: Mental and physical health are equal components to a holistic view of wellness and human thriving. Mental health should not be ignored, dismissed, or demeaned. If you find yourself struggling with mental health please visit https://www.suu.edu/mentalhealth for resources. There is also a link prominently on the right side of every Canvas page.

ADA Policy: Students with medical, psychological, learning, or other disabilities desiring academic adjustments, accommodations, or auxiliary aids will need to contact the Southern Utah University Coordinator of Services for Students with Disabilities (SSD), in Room 206F of the Sharwan Smith Center or phone (435) 865-8022. SSD determines eligibility for and authorizes the provision of services.

Emergency Management Statement: In case of emergency, the university's Emergency Notification System (ENS) will be activated. Students are encouraged to maintain updated contact information using the link on the homepage of the *mySUU* portal. In addition, students are encouraged to familiarize themselves with the Emergency Response Protocols posted in each classroom. Detailed information about the university's emergency management plan can be found at: http://www.suu.edu/emergency

HEOA Compliance Statement: The sharing of copyrighted material through peer-to-peer (P2P) file sharing, except as provided under U.S. copyright law, is prohibited by law. Detailed information can be found at: https://help.suu.edu/article/1097/p2p-and-copyright-infringement

LINK Statement: SUU faculty and staff care about the success of our students. In addition to your professor, numerous services are available to assist you with the achievement of your educational goals. SUU's LINK system may be used by faculty to notify you and/or your advisors of their concern for your progress and provide references to campus services as appropriate.

SUUSA Statement: As a student at SUU, you have representation from the SUU Student Association (SUUSA) which advocates for student interests and helps work as a liaison between the students and the university administration. You can submit My SUU Voice feedback by going here: https://www.suu.edu/suusa/voice Likewise, you can learn more about SUUSA's Executive Council here (https://www.suu.edu/suusa/executive-council/) and about individual SU-USA's Student Senators here (https://www.suu.edu/suusa/senate/)

Land Acknowledgement Statement SUU wishes to acknowledge and honor the Indigenous communities of this region as original possessors, stewards, and inhabitants of this Too'veep (land), and recognize that the University is situated on the traditional homelands of the Nung'wu (Southern Paiute People). We recognize that these lands have deeply rooted spiritual, cultural, and historical significance to the Southern Paiutes. We offer gratitude for the land itself, for the collaborative and resilient nature of the Southern Paiute people, and for the continuous opportunity to study, learn, work, and build community on their homelands here today. Consistent with the University's ongoing commitment to equity, diversity, and inclusion, SUU works towards building meaningful relationships with Native Nations and Indigenous communities through academic pursuits, partnerships, historical recognitions, community service, and student success efforts.

Disclaimer: Information contained in this syllabus, other than the grading, late assignments, make up work and attendance policies, may be subject to change as deemed appropriate by the instructor.