CHEM 301 - Physical Chemistry I
Fall 2018 Syllabus

Instructor: Nathanael M. Kidwell
Office: ISC 1287, (757)221-1701
Email: nmkidwell@wm.edu
Office Hours: Mondays at 11:00 - 12:00 pm; or by appointment or drop by
TA: Jacob Blackshaw; kjblackshaw@email.wm.edu

Course Information
Class Meetings: MWF 9:00 - 9:50 am
Class Location: McGlothlin 20
Website: Course information will be posted on Blackboard

Student Accessibility Services

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Course Description and Goals

Gilbert N. Lewis once defined Physical Chemistry as "anything that is interesting", and still remains the most accurate description of this diverse and fascinating field. This course is the first part of a two-semester introduction to Physical Chemistry, wherein both courses offer complementary approaches to the fundamental understanding of chemical systems. The microscopic (or molecular) perspective taken in CHEM 301 builds on atomic and molecular models to predict macroscopically observable properties. In particular, we will discuss two main themes during this course including quantum mechanics and spectroscopy. Learning objectives emphasized in CHEM 301 involve developing an understanding of quantum mechanical principles, and applying these principles to master the underlying concepts of electronic structure for atoms and molecules along with rotational, vibrational, and electronic spectroscopy. Linking material learned in class to modern physical chemistry techniques and research will be highlighted to give you opportunities to see how Physical Chemists are solving current, real-world problems.

Prerequisites

This is a math-intensive course, and it is expected that students have previous experience with calculus. In addition to having taken through General Chemistry II (CHEM 205 or 208), students should be familiar with the concepts learned in multivariable calculus (MATH 212 or 213) and in calculus-based physics (PHYS 101, 101L, 102, and 102L). We will review some mathematical principles along the way so that you can focus on learning the physical chemistry material.

Required Text

Physical Chemistry – A Molecular Approach by Donald A. McQuarrie and John D. Simon; University Science Books: California, 1997. ISBN: 0-935702-99-7.

Deadlines

Add/Drop Deadline: 09/07
Withdraw Deadline: 10/26

Course Structure and Grading

Problem Sets (14%) – 15 points each

There is no better way to master Physical Chemistry than by solving problems. The essence of this subject demands connecting abstract mathematical ideas with the experimentally observed behavior of chemical systems. Therefore, **nine (9) problem sets** will be posted on Blackboard due in class on the specified date. **Late work will not be accepted.** Working together in study groups of 3-4 students is encouraged as a helpful and enjoyable way to overcome conceptual obstacles and share the satisfaction of gained understanding. In reality, at the heart of good science is collaboration, so work together with your colleagues to solve problems. Groups will turn in a single, shared document bearing the names and signatures of all participants. By signing, you agree that you are seeking shared and equal credit for the assignment. Problem sets will be graded for completion and accuracy, and solutions made available on Blackboard.

Midterm Exams (61%) – 200 points each

There will be four (4) in-class midterm exams given during the semester, each worth 20% of the course point total. Midterm exam dates and tentative exam coverage are as follows:

Midterm Exam 1	Mon 09/24	Dawn of QM – Postulates of QM
Midterm Exam 2	Fri 10/12	Harmonic Oscillator – Rigid Rotor
Midterm Exam 3	Mon 11/05	H-Atom – Chem. Bonding (MO Theory)
Midterm Exam 4	Wed 11/28	Chem. Bonding (Hetero.) – Elect. Spect.

The lowest midterm exam score will be dropped, leaving 3 midterm exams in total that comprise 61% of the total course points.

Final Exam (25%) – 250 points

A comprehensive, final exam will be given on Mon, 12/10 from 9:00 am – 12:00 pm.

To receive a grade in the A range in this course, you must have at least 90%; the B range is at least 80%; the C range is at least 70%, and the D range is at least 60%. These thresholds may be lowered (i.e., it may become easier to get a higher grade), but they will not be raised.

Help Sessions

Help Sessions: On Thursday evenings from 7:00 – 8:00 pm, there will be an optional help session in ISC 1221. This time will be used to review mathematical concepts and classroom material. Key aspects of Help Sessions will include active dialogue between the professor and students as well as communication and problem-solving.

Helpful Resources:
(1) *Applied Mathematics for Physical Chemistry*, 3rd Edition by James R. Barrante; Pearson Prentice Hall: 2012. ISBN: 978-0131008458.
(2) *Physical Chemistry*, 3rd Edition by Thomas Engel and Philip Reid; Prentice Hall: New York, 2013. ISBN: 1-292-02224-8.

Poll Everywhere

Poll Everywhere (PollEv) is a student response system that works on any internet-enabled device (e.g., laptop, cell phone, etc.), and is free for William & Mary students. We will be using Poll Everywhere during lectures to create an interactive and engaging learning environment, where both students and the instructor are active participants in the classroom discussion. This will allow me to instantly take the "classroom's temperature" by prompting questions that assess current understanding of the material or raising open-ended discussion questions. Questions using Poll Everywhere will not be graded, but it is in your best interests to participate to gauge for yourself how well you know the material.

Students can create an account using their William & Mary credentials by visiting https://www.polleverywhere.com/login. Upon entering a William & Mary student email address, users will be prompted to sign in via Single-Sign On (SSO). Students can access this course's PollEv site either (a) through the app using PollEv.com/CHEM301 or (b) through an online browser at https://pollev.com/CHEM301

Policies

Email: I will make every effort to respond to emails promptly. **When you email me, please put CHEM 301 in the subject line.** In order to encourage you to proactively prepare for exam and problem set due dates, I reserve the right not to answer last minute emails that are received after 5:00 pm the night before an exam or problem set due date.

Make-up Policy: No make-up exams will be given without (a) pre-arranging this with me **well before** the day of the exam **OR** (b) providing documentation demonstrating a medical emergency. It is in your best interests to arrive late for an exam, rather than skipping it altogether! No extensions will be given for problem sets.

Classroom Expectations: Every student is entitled to a classroom environment that is conductive to learning. You are expected to refrain from any behavior that disrupts

the learning environment. Please respect other students and the professor by arriving on time and staying until the end of class. As a courtesy to your fellow classmates, do not surf the web or text message during the class, or you will be asked to leave. On the contrary, it is critical that you are actively participating and contributing to the classroom discussion. Make wise use of your time!

Exams: For each midterm and final exam, you will be allowed to bring a scientific calculator, and pencils or pens. Use of computers, cell phones, or any other type of electronic device is prohibited during exams.

Problem Sets: You may work on homework with other students, but directly copying each other's work is academic misconduct.

How to Succeed in Physical Chemistry

1) **Come to class prepared:** Read through the notes from the previous class as each lecture builds off of each other. During the lecture, actively think about how all of the concepts fit together, and how the material covered today relates to what was discussed in the previous class. Be ready to work problems and talk about physical chemistry with your neighbors. **Ask questions!**
2) **Study actively:** Rework in-class problems at home without having the solutions in front of you. Work and rework the homework problems to prepare yourself for the exams. Read through your class notes and actively thinking about how all of the concepts fit together, why they make sense, and what is confusing to you. Much of physical chemistry is about learning how to problem solve and thinking critically about abstract concepts. In my experience, the best way to build these skills is to actively practice **DOING** them!
3) **Form study groups**: This is challenging material – don't tackle it alone! I fully encourage everyone to study in groups as so much learning can take place when a group is collectively thinking about and talking through problems!
4) **Stop and think about the chemistry**: There is a lot of math in physical chemistry and it can be easy to get lost in all of the equations and lose sight of what it all physically means. As you're working through a problem or trying to understand some equations, stop and think about what scientific concepts are involved and what all of the math tells you about the world around us. If you're unclear, ask me or a fellow student!
5) **Come to office hours**: My goal is to use office hours as an interactive recitation where we can all discuss questions about lecture as well as the upcoming problem set. As such, it will likely be beneficial to regularly attend office hours.
6) **Read**: After lecture, read through your lecture notes and fill-in any key information you may have missed. Supplement the lecture notes by reading pertinent sections of the required and/or recommended texts.
7) **Budget your time**: Do **NOT** wait until the night before a problem set is due to start working on it! Study for the exams throughout the semester, not just right before they occur!

Course Schedule*

Date	Topics	Reading	Assignment Due
8/29	The Dawn of Quantum Mechanics		
8/31	The Dawn of Quantum Mechanics	1-1 to 1-3, 1-6, 1-7	
9/3	The Classical Wave Equation	2-1 to 2-3	
9/5	The Schrödinger Equation	3-1 to 3-3	Problem Set 1
9/7	1-D Particle in a Box	3-4 to 3-7	
9/10	1-D Particle in a Finite Box	Handouts	
9/12	3-D Particle in a Box	3-9	Problem Set 2
9/14	Postulates of Quantum Mechanics	4-1 to 4-3	
9/17	Postulates of Quantum Mechanics	4-3 to 4-6	
9/19	Harmonic and Anharmonic Oscillator	5-1 to 5-3	Problem Set 3
9/21	Harmonic Oscillator: Energy Levels	5-4, 5-5	
9/24	**Midterm Exam I**		
9/26	Harmonic Oscillator: Wave Functions; Tunneling	5-6, 5-7	
9/28	Anharmonic Oscillator: Energy Levels and Bond Breaking	5-3	
10/1	Rigid Rotor: Energy Levels; Wave Functions	5-8	Problem Set 4
10/3	Rigid Rotor: Diatomic Molecules	5-9	
10/5	Hydrogen Atom: Schrödinger Equation; Wave Functions	6-1, 6-2	
10/8	Hydrogen Atom: Angular Momentum; Quantum Numbers	6-3, 6-4	Problem Set 5
10/10	Hydrogen Atom: Orbitals; Helium Atom	6-5 to 6-7	
10/12	**Midterm Exam 2**		
10/15	**Fall Break - No Class**		
10/17	Multielectron Atoms: Theoretical Methods	8-1 to 8-3	
10/19	Multielectron Atoms: Spin	8-4 to 8-7	
10/22	Multielectron Atoms: Atomic Term Symbols; Hund's Rules	8-8 to 8-11	
10/24	Chemical Bonding: H_2, H_2^+, Orbital Overlap	9-1 to 9-5	Problem Set 6
10/26	Chemical Bonding: Molecular Orbital Theory	9-6 to 9-11	
10/29	Chemical Bonding: Molecular Orbital Theory	9-6 to 9-11	
10/31	Chemical Bonding: Heteroatomics; LCAO; Molecular Term Symbols	9-12 to 9-16	Problem Set 7
11/2	Chemical Bonding: Heteroatomics; LCAO; Molecular Term Symbols	9-12 to 9-16	
11/5	**Midterm Exam 3**		
11/7	Molecular Spectroscopy Overview; Rotational Spectroscopy	13-1, 13-2, 13-4	
11/9	Rotational Spectroscopy	13-8, 13-12	
11/12	Vibrational Spectroscopy	13-3, 13-5	Problem Set 8
11/14	Vibrational Spectroscopy	13-9, 13-13	
11/16	Electronic Spectroscopy	13-6	
11/19	Electronic Spectroscopy	13-7	Problem Set 9
11/21	**Thanksgiving Holiday**		
11/23	**No Classes**		
11/26	Wrap-Up: Bringing It All Together		
11/28	**Midterm Exam 4**		
11/30	Special Topics		

Course Schedule Cont'd*

Date	Topics	Reading	Assignment Due
12/3	Special Topics		
12/5	Review		
12/7	Review		
12/10	**Final Exam; 9am-12pm**		

* This schedule is tentative and is subject to change.