SYLLABUS

Introduction:

All of chemistry, including bonding, reactions, thermodynamics, kinetics, and material properties, ultimately emerges from the motion and behavior of atoms and molecules. Quantum mechanics, a model to describe this motion and behavior, is one of the most accurate and fruitful theoretical frameworks in the history of science. *The value in knowing quantum mechanics comes from its predictive power*. The better you know quantum mechanics, the better you will understand what causes the atoms to act the way they do that results in the chemistry that we observe and use.

Course: **Chemistry 3026:** Physical Chemistry II – Quantum Chemistry and Molecular Spectroscopy

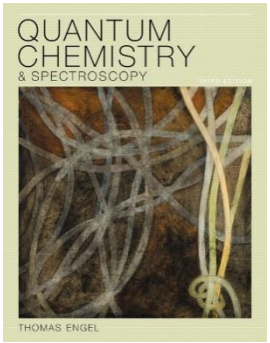
T,Th 9:30 – 10:45 AM in Latter Hall room 102

Instructor: Dr. Lane Votapka
Office location: Rohr Science room 322
Office hours: MWF 2:45 – 5:00 PM and by appointment
Phone: 619-849-2270
Email: lvotapka@pointloma.edu
(I will be able to answer emails between 8 AM and 6 PM).

Text: Quantum Chemistry & Spectroscopy, Third Edition, Thomas Engel, Pearson Education, 2013.

Course Description: Study of reaction dynamics and complex reaction mechanisms and an investigation of matter from a quantum chemistry perspective with particular emphasis on the theoretical concepts and their implications for molecular spectroscopy.

Course Learning Outcomes: Upon completing this course you will:



1. Have developed more sophisticated mental models of wave functions, energy levels, atomic structures, chemical bonding, spectroscopy, computational chemistry, and statistical mechanics as grounded in the fundamentals of quantum theory.
2. Be able to use fundamental exact and approximate physical systems as models for understanding more complex molecular structure and behavior.
3. Be able to apply the concepts, methods, and techniques of quantum chemistry to chemical systems and make predictions for these systems.

Homework & Quizzes: Assignments will be essential to the learning process of this course's content; therefore, problems sets will be assigned regularly. There will be three types of assignments:

- Homework problems: each problem will be graded with a +, ✓, –, or a 0, which corresponds to 150%, 100%, 50%, and 0% credit, respectively, for each problem and you may collaborate with other students on these problems.
- Worksheets will be handed out in class and will often refer to an online video or other resource in order to practice mathematical derivations or expand understanding on a particular topic. They will be collected and graded at a later time.
- Quizzes will be held periodically in class and will mimic problems of the type that will be encountered on the exams.

I am available in office hours to help with homework and worksheet problems. All homework and worksheets must be turned in by the beginning of class on the assigned due date. Usually homework will be due every Thursday.

Participation: Discussions and collaboration with your fellow student "colleagues" will be very helpful to facilitate everyone's understanding of quantum mechanics. Small-group activities and problem-solving will be conducted frequently in class. Your participation score will be assigned based on engagement in class.

To minimize distractions to both yourself and others, please don't use laptops or phones in class. It would be nearly impossible to takes notes on quantum mechanics using a laptop anyways.

Attendance: Regular and punctual attendance at all classes is considered essential to optimum academic achievement. If the student is absent from more than 10 percent of class meetings, the faculty member can file a written report which may result in de-enrollment. If the absences exceed 20 percent, the student may be de-enrolled without notice until the university drop date or, after that date, receive the appropriate grade for their work and participation. See Academic Policies in the Undergraduate Academic Catalog.

Assessment and Grading:

Mid-term exam 1	20%
Mid-term exam 2	20%
Final exam	25%
Homework	10%
Quizzes	15%
Worksheets	5%
Participation	5%

A	90%	C	70%
A-	88%	C-	68%
B+	86%	D+	66%
B	80%	D	60%
B-	78%	D-	58%
C+	76%	F	< 58%

PLNU Mission

To teach ~ to shape ~ to send

Point Loma Nazarene University exists to provide higher education in a vital Christian community where minds are engaged and challenged, character is modeled and formed, and service is an expression of faith. Being of Wesleyan heritage, we strive to be a learning community where grace is foundational, truth is pursued, and holiness is a way of life.

Course Credit Hour Information

In the interest of providing sufficient time to accomplish the state Course Learning Outcomes, this class meets the PLNU credit hour policy for a 3 unit class delivered over 16 weeks. Specific details about how the class meets the credit hour requirement can be provided upon request.

Final Examination Policy

Successful completion of this class requires taking the final examination on its scheduled day. The final examination schedule is posted on the Class Schedules site. No requests for early examinations or alternative days will be approved.

PLNU copyright policy

Point Loma Nazarene University, as a non-profit educational institution, is entitled by law to use materials protected by the US Copyright Act for classroom education. Any use of those materials outside the class may violate the law.

PLNU Academic Honesty Policy

Students should demonstrate academic honesty by doing original work and by giving appropriate credit to the ideas of others. Academic dishonesty is the act of presenting information, ideas, and/or concepts as one's own when in reality they are the results of another person's creativity and effort. A faculty member who believes a situation involving academic dishonesty has been detected may assign a failing grade for that assignment or examination, or, depending on the seriousness of the offense, for the course. Faculty should follow and students may appeal using the procedure in the university Catalog. See Academic Policies for definitions of kinds of academic dishonesty and for further policy information.

PLNU Academic Accommodations policy

While all students are expected to meet the minimum standards for completion of this course as established by the instructor, students with disabilities may require academic adjustments, modifications or auxiliary aids/services. At Point Loma Nazarene University (PLNU), these students are requested to register with the Disability Resource Center (DRC), located in the Bond Academic Center. (DRC@pointloma.edu or 619-849-2486). The DRC's policies and procedures for assisting such students in the development of an appropriate academic adjustment plan (AP) allows PLNU to comply with Section 504 of the Rehabilitation Act and the Americans with Disabilities Act. Section 504 (a) prohibits discrimination against students with special needs and guarantees all qualified students equal access to and benefits of PLNU programs and activities. After the student files the required documentation, the DRC, in conjunction with the student, will develop an AP to meet that student's specific learning needs.

The DRC will thereafter email the student's AP to all faculty who teach courses in which the student is enrolled each semester. The AP must be implemented in all such courses.

If students do not wish to avail themselves of some or all of the elements of their AP in a particular course, it is the responsibility of those students to notify their professor in that course. PLNU highly recommends that DRC students speak with their professors during the first two weeks of each semester about the applicability of their AP in that particular course and/or if they do not desire to take advantage of some or all of the elements of their AP in that course.

Class Schedule –Tentative--:

Sessions	**Topics**	**Readings**
Sept 5	Introduction: From Classical to Quantum Mechanics	Chapter 1, sections 1.1-1.7
Sept 5 1PM-5PM	Calculus boot camp	
Sept 10, 12	The Schrödinger Equation	Chapter 2, sections 2.1-2.8
Sept 17	The Quantum Mechanical Postulates	Chapter 3, sections 3.1-3.5
Sept 19, 24	Using Quantum Mechanics on Simple Systems	Chapter 4, sections 4.1-4.4
Sept 26	The Particle in a Box and the Real World	Chapter 5, sections 5.1-5.3,5.5-5.6
Oct 1, 3	Commuting and Non-commuting Operators	Chapter 6, sections 6.1, 6.3-6.5
Oct 8	**Midterm Exam 1 (Chapters 1-6)**	
Oct 10, 15	Models for the Vibrations and Rotations of Molecules	Chapter 7, sections 7.1-7.7
Oct 17	The Vibrational and Rotational Spectroscopy of Diatomics	Chapter 8, sections 8.1-8.6
Oct 22, 24	The Hydrogen Atom	Chapter 9, sections 9.1-9.6
Oct 29, 31	Many-Electron Atoms	Chapter 10, sections 10.1-10.6 (also section 6.2)
Nov 5	Quantum States for Many-Electron Atoms and Atomic Spectroscopy	Chapter 11, sections 11.1-11.4, 11.11
Nov 7, 12	The Chemical Bond in Diatomic Molecules	Chapter 12, sections 12.1-12.9
Nov 14	**Midterm Exam 2 (Chapters 7-12)**	
Nov 19, 21	Molecular Structure and Energy Levels for Polyatomic Molecules	Chapter 13, sections 13.1-13.2, 13.4-13.5, 13.7
Nov 26	Electronic Spectroscopy	Chapter 14, sections 14.1-14.4, 14.6-14.8
Dec 3, 5	Computational Chemistry	Chapter 15, sections 15.1-15.8, 15.10
Dec 10, 12	Molecular Symmetry	Chapter 16, sections 16.1-16.4
Dec 17, 10:30 AM – 1:00 PM	**Comprehensive Final Exam** Final Exam: Tues. Dec 17, 10:30 AM – 1:00 PM, Latter Hall room 102	