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 326:** Physical Chemistry II – Quantum Chemistry and Molecular Spectroscopy

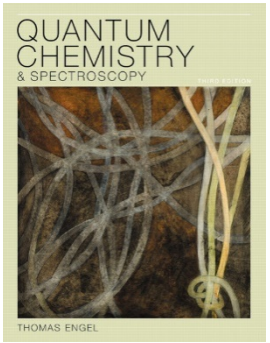
MWF 8:30 – 9:25 AM in Ryan Learning Center room 102

Instructor: Dr. Lane Votapka
Office location: Rohr Science room 305E
Office hours: MWF 10:30 – 12:00
Thursday 11-12:30 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: An investigation of matter from a quantum chemistry perspective with particular emphasis on the theoretical concepts and their implications for molecular spectroscopy.

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: Homework will be essential to the learning process of this course's content; therefore, problems sets will be assigned regularly. Each assignment will be composed of two types of problems:

- Work problems: each problem will be graded with a +, ✓, or –, and you may collaborate with other students on these problems.
- Quiz problems are mini take-home exams and you are all expected to do them individually.

I am available to help with both types of problems.
All homework and quizzes must be turned in by the beginning of class on the assigned due date. Usually homework and quizzes will be due every Wednesday.

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. Online forums will be utilized for discussion. Your participation score will be assigned based on engagement in both in-class as well as online discussions.

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.

Grading:

Mid-term exam 1	20%
Mid-term exam 2	20%
Final exam	25%
Homework	15%
Quizzes	15%
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.

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

If you have a diagnosed disability, please contact PLNU's Disability Resource Center (DRC) within the first two weeks of class to demonstrate need and to register for accommodation by phone at 619-849-2486 or by e-mail at DRC@pointloma.edu. See Disability Resource Center for additional information.

Class Schedule –Tentative--:

Sessions	**Topics**	**Readings**
Aug 29, 30	Introduction: From Classical to Quantum Mechanics	Chapter 1, sections 1.1-1.7
Aug 31	Special topic session (2-5pm in Latter 101)	
Sept 1, 6, 8	The Schrödinger Equation	Chapter 2, sections 2.1-2.8
Sept 11, 13	The Quantum Mechanical Postulates	Chapter 3, sections 3.1-3.5
Sept 15, 18	Using Quantum Mechanics on Simple Systems	Chapter 4, sections 4.1-4.3
Sept 20, 22	The Particle in a Box and the Real World	Chapter 5, sections 5.1-5.3,5.5-5.6
Sept 25, 27, 29	Commuting and Non-commuting Operators	Chapter 6, sections 6.1, 6.3-6.5
Oct 2	**Midterm Exam 1 (Chapters 1-6)**	
Oct 4, 6, 9	Models for the Vibrations and Rotations of Molecules	Chapter 7, sections 7.1-7.7
Oct 11, 13	The Vibrational and Rotational Spectroscopy of Diatomics	Chapter 8, sections 8.1-8.6
Oct 16, 18, 23	The Hydrogen Atom	Chapter 9, sections 9.1-9.6
Oct 25, 27, 30	Many-Electron Atoms	Chapter 10, sections 10.1-10.6 (also section 6.2)
Nov 1, 3, 6	Quantum States for Many-Electron Atoms and Atomic Spectroscopy	Chapter 11, sections 11.1-11.4, 11.11
Nov 8, 10, 13	The Chemical Bond in Diatomic Molecules	Chapter 12, sections 12.1-12.9
Nov 15	**Midterm Exam 2 (Chapters 7-12)**	
Nov 17, 20	Molecular Structure and Energy Levels for Polyatomic Molecules	Chapter 13, sections 13.1-13.2, 13.4-13.5, 13.7-13.8
Nov 27, 29	Electronic Spectroscopy	Chapter 14, sections 14.1, 14.3-14.8
Dec 1, 4	Computational Chemistry	Chapter 15, sections 15.1-15.7, 15.10
Dec 6, 8	Molecular Symmetry	Chapter 16, sections 16.1-16.4
Dec 13, 7:30 – 10:00 AM	**Comprehensive Final Exam** Final Exam: Wed. Dec 13, 7:30 AM – 10:00 AM, Ryan Learning Center room 102	