CHEM 348 $\Phi\chi$ 2021	**CHEM 348 – Physical Chemistry** **Spring 2021 Syllabus**

Instructor: Fabien Goulay, CRL 465, Fagoulay@mail.wvu.edu

Lecture: CHEM348 Section 001, 3 credit hours

Pre-requisite: CHEM 346 and MATH 251. Continuation of CHEM 346

Lectures are held on Monday, Wednesday, and Friday from 9:30 am to 10:20 am on Zoom.
https://wvu.zoom.us/j/91737888796?pwd=T05oNlRWSGRVeW4yTkF0YUwwcHE4UT09
Meeting ID: 917 3788 8796
Passcode: 6MM0QUq2

Office Hours (Zoom):

Monday 10:30 am–11:30 am
Wednesday 10:30 am–11:30 am
Friday 10:30 am–11:30 am

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Meeting ID: 917 3788 8796
Passcode: 6MM0QUq2

Students unable to meet at these times due to schedule conflicts should make an appointment (via email) if a meeting is desired.

Description of the class: In this class we will describe the basic principles of physical chemistry, quantum mechanics, and molecular collision to understand, analyze, and predict the spectra and reactivity of molecules.

Learning objectives: The objectives of the course are to:

- Understand the limitations of classical mechanics that led to the development of quantum mechanics.
- Apply the postulates of quantum mechanics to 1D, 2D, and 3D motions of particles. Use the results to predict the absorption wavelength of simple unsaturated molecules.
- Write the Schrodinger equation for a particle travelling through a potential barrier and use the boundary conditions to infer the wavefunction. Calculate the transmission probability.
- Calculate the standard deviation of a measurement. Apply the Heisenberg uncertainty principle to simple translational motions.
- Have a basic knowledge of the technics of approximation used in quantum chemistry.
- Write the Schrodinger equation for the hydrogen atom, separate the variables and solve for the angular part of the wavefunction.
- Draw the orbitals and probability densities of the hydrogen atoms.
- Write the Schrodinger equation for a multi electron atom.
- Understand the orbital approximation and give the Slater determinant for small atoms.
- Calculate the first ionization energy of atoms.
- Give all the atomic term symbols associated with an atomic configuration (non-equivalent electrons).
- Draw the energy diagram and emission/absorption spectrum of atomic transitions.
- Write the Schrodinger equation for rotational and vibrational motions of molecules.
- Analyze the rotational and vibrational spectra and infer molecular properties.
- Draw the molecular energy diagram of diatomic molecules.
- Give the ground electronic state configuration and bond order.
- Have basic knowledge of the kinetic theory of gases.

Learning outcomes: After completing the course, the students will grasp the fundamental principles of quantum mechanics and be able to apply them to understand and predict the structure of atoms and diatomic molecules. The students will also be able to interpret the rotational and vibrational spectra of diatomic molecules and infer molecular properties.

Problem solving sessions: A number of problem-solving sessions will be distributed throughout the semester, likely every other Friday. Problem sets for these regular class-time sessions will be available few days in advance. The attendance policy for these sessions is the same as for regular lectures.

Textbooks

Physical Chemistry by P. W. Atkins et al., 11th Edition (Required)
and
Solution manual for physical chemistry by P. W. Atkins, et al. (Recommended)

Additional resources

Additional information may be found in the following books (NOT REQUIRED):

-*Quantum Chemistry and Spectroscopy* by T. Engel, 2nd Edition.

-*Quantum chemistry* by D. A. McQuarrie, 2nd edition, University Science Books.

-*Modern Spectroscopy* by J. M. Hollas, 4th edition (Wiley, 2009).

-*Chemical Kinetics and Reaction Dynamics* by P. L. Houston, Dover Publication.

Pre-requisite: You are expected to review the most relevant topics from mathematics before proceeding to quantum chemistry and its applications. Refer to the textbook for important mathematical background.

Differentiation .... *Chemist's toolkits 5 p 22*

Integration .... *Chemist's toolkits 4 p 14*

Partial derivatives .... *Chemist's toolkits 9 p 44*

Complex numbers .... *Chemist's toolkits 14 p 247*

Integration by parts .... *Chemist's toolkits 15 p 254*

Euler's formula .... *Chemist's toolkits 16 p 256*

Cylindrical coordinates .... *Chemist's toolkits 19 p 281*

Spherical polar coordinates .... *Chemist's toolkits 21 p 286*

Matrices .... *Chemist's toolkits 24 p 373*

Additional information can be found in "*Mathematics for Physical Chemistry*" D. A. McQuarrie, University Science Books.

Grading

Grades are based on performance assessments that reflect achievement of learning outcomes outlined for this course.

Grade Formulation:

Homework (7)	350 points
Exams (2)	400 points
Final Exam (1)	250 points

The exams account for 40.0%, the final accounts for 25.0%, the homework assignments for 35.0% of the total grade. 100 (10%) extra credit points will be distributed among the homework assignments and exams.

Important dates:

01/20	First day of class	04/02	*Spring Holiday*
01/25	Due date Homework 1	04/09	Due date Homework 6
02/05	Due date Homework 2	04/12	Exam 2
02/19	Due date Homework 3	04/23	Due date Homework 7
03/01	Exam1	05/01	Last day of class
03/03	No class	05/04–05/08	Final Exam Week
03/12	Due date Homework 4	**05/05**	**Final Exam 2-4pm**
03/26	Due date Homework 5		

Lecture: It is important that you take notes during lecture, which are legible and organized. Your notes will become your most important study material for the examinations. **You must review your notes before the next class**, this will prevent you from being "lost" during the lecture period. Read the textbook assignments after the class period for which they are assigned.

Homework assignments: Students will be given several homework assignments during the semester. They will be assigned at least one week before the due date. In order to receive credit, students must provide full detail, including unit analysis, mathematical derivation, and insightful justification unless otherwise noted. Carry units through your work and clearly indicate your result in a box. Illegible work will be given a score of 0 %. Material covered on these assignments may differ from the lecture in order to encourage critical thinking and problem-solving skills. Turn in your assignments clearly labeled with your name and problem numbers. On due dates, the problem sets can be turned electronically by the end of the day (5 PM). See "*Instructions to submit homework assignments*" for details. Late homework assignments will not be accepted.

Exams: Two 50-min exams will be given during the term. A variety of problems will be included on each exam. Material covered on the exams will be taken mainly from the lecture and assigned problems. Specific instructions will be given for each exam.

Final Examination: The final examination will be comprehensive and cumulative, covering the entire course. Your study during the semester should be designed for comprehensive and long-term retention of the factual material, principles, and their application. Specific instructions will be given for the final exam.

Make-up Policy: Absences/makeups will be dealt with on an individual basis. Please contact the instructor as soon as possible. No make-up exams will be given after the test has been discussed in class. Homework assignments are due on the specified date. Extensions will be given for appropriately excused absences as outlined above.

Attendance: Attendance is mandatory for CHEM 348. Poor attendance during the semester may result in a lower letter grade for the class.

<u>**Tentative Course Outline**</u>	***Topic in Atkin's 11th edition***
Part A Fundamentals of Quantum Chemistry	
Chapter 0 Science at the end of the 19th century	Reviews
Chapter 1 From classical to quantum	7A
1.1 The black body radiation	
1.2 The photoelectric effect	
1.3 Atomic spectra and the Bohr model of the atom	
1.4 Particle wave	
1.5 Classical vs. quantum mechanics	
Chapter 2 Quantum mechanical postulates	7B, 7C.1(a), (b), 7C.2, 7C.4
2.0 Definition of a postulate	
2.1 The physical meaning of the wave function	
2.2 Every observable has a corresponding operator	
2.3 The result of an individual measurement	
2.4 The expectation value	
2.5 The time evolution of a quantum mechanical system	
Chapter 3 The Schrodinger equation and its solutions	7B.1, 7D
3.1 Time dependent and time independent equations	
3.2 Solving the Schrodinger equation	
3.3 Properties of quantum mechanical eigenfunctions	
3.4 The particle in a box	
3.5 Quantum Tunnelling	
Chapter 4 The uncertainty principle	7C.3
4.1 Commuting operators	
4.2 Momentum and position operators	
4.3 Standard deviation	
4.4 Heisenberg uncertainty principle	
Chapter 5 Techniques of approximation	9D.2
5.1 Variation theory	
5.2 Perturbation theory	
Part B Atomic and Molecular Structures	
Chapter 1 The hydrogen atom	8A, 8.B.2(a)
1.0 Spherical coordinates	
1.1 The Schrodinger equation for the one-electron atom	
1.2 Eigenvalues and eigenfunctions of the H atom	
1.3 The hydrogen atom orbitals	
1.4 The electron spin	
Chapter 2 Many electron atoms	8B
2.1 The orbital approximation	
2.2 The Pauli principle	
2.3 Trends in the periodic table	
2.4 Atomic term symbols	
Chapter 3 Introduction to spectroscopy	8C
3.1 Light–matter interaction	
3.2 Spectroscopic selection rules	
3.3 Application to atomic spectroscopy	
Chapter 4 Vibration and rotation of molecules	7E, 7F, 11B, 11C, 11D
4.2 Pure rotational spectroscopy of linear molecules	
4.3 The harmonic oscillator	
4.4 Rovibrational spectroscopy of diatomic molecules	
Chapter 5 Molecular orbital theory	9B, 9C, 9D
5.1 Variation theory and orbital overlap	
5.2 Molecular energy diagram of diatomic molecules	
5.3 Rovibronic spectroscopy of diatomic molecules	
Part C Molecular Dynamics	
Chapter 1 Kinetic theory of gasses	1B
1.1 Pressure and energy of an ideal gas	
1.2 The Maxwell distribution of speeds	
1.3 Mean free path and collision number	
Chapter 2 Reactive collisions	18A
2.1 The thermal reaction rate	
2.2 Reaction with an activation energy	

Syllabus Statements

Inclusivity Statement: The West Virginia University community is committed to creating and fostering a positive learning and working environment based on open communication, mutual respect, and inclusion. If you are a person with a disability and anticipate needing any type of accommodation in order to participate in your classes, please advise your instructors and make appropriate arrangements with the Office of Accessibility Services. (https://accessibilityservices.wvu.edu/) More information is available at the Division of Diversity, Equity, and Inclusion (https://diversity.wvu.edu/ as well. [adopted 2-11-2013]

Academic Integrity Statement: The integrity of the classes offered by any academic institution solidifies the foundation of its mission and cannot be sacrificed to expediency, ignorance, or blatant fraud. Therefore, instructors will enforce rigorous standards of academic integrity in all aspects and assignments of their courses. For the detailed policy of West Virginia University regarding the definitions of acts considered to fall under academic dishonesty and possible ensuing sanctions, please see the West Virginia University Academic Standards Policy. Should you have any questions about possibly improper research citations or references, or any other activity that may be interpreted as an attempt at academic dishonesty, please see your instructor before the assignment is due to discuss the matter.

Appropriate Use of Technology Statement: Use of technology in the classroom should always be directly related to class activities and/or course learning outcomes. Inappropriate technology use can be an impediment to learning and a distraction to all members of the class. As such, inappropriate use of technology in the classroom may be considered a disruption of the class and constitute a violation of the WVU Student Conduct Code and could potentially result in a referral to the Office of Student Conduct. Use of technology in the classroom when specifically prohibited by the instructor may also constitute a violation of WVU's Academic Integrity policy.