Physical Chemistry I
(CHEM 4300)

Autumn Semester 2019
Lectures: MWF 1:50 - 2:45 pm, CBEC 130

Instructor: Alexander Sokolov
E-mail: sokolov.8@osu.edu
Office: 2108 Newman Wolfrom Lab
Office hours: Wed. 5:00 - 6:00 pm, Fri. 4:00 - 5:00 pm or by appointment
The office hours will take place in the instructor's office, 2108 Newman Wolfrom Lab. Occasionally the time of office hours will need to be moved, and these changes will be announced in class. There may be a few days when Dr. Sokolov will not be able to attend office hours. This will be announced in class and and extra office hours will be scheduled if needed by the class.

Recitations:

Recitation	TA	Email	Room
Mon. 4:10 - 5:05 pm	Justin Seffernick	seffernick.9@osu.edu	McPherson Lab 1021
Tues. 8:00 - 8:55 am	Samragni Banerjee	banerjee.156@osu.edu	Bolz Hall 313
Tues. 3:00 - 3:55 pm	Samragni Banerjee	banerjee.156@osu.edu	Enarson Classroom Bldg 318
Tues. 4:10 - 5:05 pm	Justin Seffernick	seffernick.9@osu.edu	McPherson Lab 1035

Recitation sessions will be a time for the teaching assistants to go over material from lecture, math background, review for exams or answer questions on problem sets. Closed book quizzes will be given during the last 20 minutes of four recitations, according to the schedule given in the syllabus (see below). **You may not attend a recitation other than the one for which you are registered.**

TA's office hours:

TA	Email	Office hour	Room
Samragni Banerjee	banerjee.156@osu.edu	Wed. 4:00 - 5:00 pm	Macquigg 162
Samragni Banerjee	banerjee.156@osu.edu	Thur. 12:00 - 1:00 pm	Caldwell 102
Justin Seffernick	seffernick.9@osu.edu	Wed. 10:00 - 11:00 am	Derby 062
Justin Seffernick	seffernick.9@osu.edu	Thur. 3:00 - 4:00 pm	Watts 0389

You may attend any one (or all) of the TA's office hours.

Course description:
Classical mechanics accurately predicts the motion of objects we encounter in our everyday world: basketballs, cars, planets, etc. It completely fails for atomic and sub-atomic particles like electrons. Yet the motion of electrons and nuclei is what determines the course of chemical reactions. Therefore, to understand chemistry, you have to understand the correct theory for the motion of atomic particles, namely quantum mechanics.

The expected learning outcome for CHEM 4300 is for you to grasp how motion is described in quantum mechanics using a wave function, instead of the variables of classical mechanics, like position and velocity. You will study quantum behavior in a few essential physical systems – the free particle, particle confined in a "box", the harmonic oscillator, rigid rotator, and the hydrogen atom. Beyond these simple systems, one must either rely on approximate solutions of quantum

equations of motion, or employ computational methods. You will learn how quantum mechanics can describe chemical bonding. Moving beyond quantum mechanics, you will begin to study the fundamentals of molecular kinetic theory and chemical kinetics.

The broader goal of this course is to provide you with the skill to use the language of mathematics to describe natural phenomena, as well as the ability to apply this skill in a variety of different contexts. This will enable you to effectively engage with the scientific community and absorb quantitative aspects of the scientific literature.

Textbook:
"Physical Chemistry, A Molecular Approach" by Donald A. McQuarrie and John D. Simon

Topics:
We will be covering the material from McQuarrie and Simon's textbook. Below is the approximate timeline that will be adjusted as necessary throughout the semester.

Approx. Dates	Topics	Reading
On Your Own	Classical Wave Equation	Ch. 2
Aug. 21 - 23	Historical Setting	Ch. 1, Math Ch. A, B
Aug. 26 - 30	Postulates and Fundamentals of Quantum Mechanics	Ch. 4, Math Ch. C
Sept. 4 - 11	Particle in a Box and Some Important Features of Quantum Mechanics	Ch. 3
Sept. 13- 18	Model Systems: Harmonic Oscillator, Rigid Rotator	Ch. 5, Math Ch. D
Midterm 1: Friday, September 20, in class		
Sept. 23 - Oct. 2	Angular Momentum and the Hydrogen Atom	Ch. 6
Oct. 4 - 9	Approximation Methods	Ch. 7, Math Ch. E
Midterm 2: Friday, October 18, in class		
Oct. 14 - 23	Multielectron Atoms	Ch. 8
Oct. 25 - Nov. 4	Chemical Bonding: Diatomic and Polyatomic Molecules	Ch.'s 9 and 10
Nov. 6	Computational Chemistry	Ch. 11
Nov. 8-15	Molecular Spectroscopy	Ch.'s 13, 14
Midterm 3: Monday, November 18, in class		
Nov. 20 - Dec. 2	Chemical Kinetics – Rate Laws and Reaction Mechanisms	Ch.'s 28, 29
Dec. 4	Review Session	

There will be no classes, office hours, or recitations on Monday Sept. 2 in observation of Labor Day, Oct. 10-11 due to Autumn Break, Nov. 11 in observance of Veterans Day, and Wednesday Nov. 27 through Friday Nov. 29 in observance of Thanksgiving.

Grading:
Homework: 10%
Quizzes: 10%
Midterm 1: 20%
Midterm 2: 20%
Midterm 3: 20%
Final Exam: 20%

The teaching assistants are responsible for all grading. They will design grading rubrics and

consistently grade according to those. One TA will grade a problem for the entire class. If you have a question regarding grading on some of your work, identify the TA who graded this problem and talk to them. **For the sake of consistency, the instructor will not overrule TA decisions, unless they were plain wrong**.

Molecular quantum mechanics and chemical kinetics are tough subjects, so no one expects perfection, not even from A students. Our goal is that all students come away from this course with a good understanding of molecular quantum mechanics and chemical kinetics. When assigning the final grades, the instructor will look over your graded materials, and come to a judgment as to what the grades are telling him. Those students who have a strong command of most of the material will get an A.

Exams:
There will be three midterm exams and a final exam. The date, time, and place of the final exam will be announced in class and on Carmen. The midterm exams will be given at the following times:

Midterm 1: Friday, September 20, in class (1:50 - 2:45 pm)
Midterm 2: Friday, October 18, in class (1:50 - 2:45 pm)
Midterm 3: Monday, November 18, in class (1:50 - 2:45 pm)

Exams will be closed book. Generally, no aides are permitted during the exam. Any material that is out will be considered academic misconduct. The instructor will inform you whether you will be permitted to bring a non-graphing calculator.

There should be no conflicts with these exam dates as they are given in class. However, if you have a conflict with any of the exams, please let Dr. Sokolov know as soon as possible to determine whether you are eligible for an alternate exam.

Homework:
After listening to a lecture and reading the text, the learning process is completed by actively writing out problem solutions. That is why we place emphasis on working on practice problems as much as possible in active mode (thinking about the problem yourself) rather than passive mode (being told the solutions by a TA, the instructor, or your classmates). Of course, when you attempt the problems independently you will get stuck on some problems and need help, but when that happens you will learn something. The more passive you are, the less you will learn. Homework problems may be discussed with anyone, but assignments must be written up individually and must represent your own work. The submitted work should reflect the student's level of understanding.

Weekly homework problems will count for 10% of your final grade. It is in your interest to make sure your work is legible and your reasoning is clear. Please be sure to include your name and your recitation section (TA name) and staple all your work. Points will be deducted for missing names, sections (TA name) and loose paperwork. Please write on both sides of the paper. Homework assignments are due at the beginning of class on due date (listed on the assignment, also see below), and have to be turned in in class. Late assignments will not be accepted without prior permission of the instructor. Solutions for the homework will be posted on Carmen.

Problem sets must be turned in in class before the beginning of class on due date (i.e., by 1:50 pm). These deadlines may only be changed by the instructor. Unless changed by the instructor, problem sets will be due on:

Homework 1: Aug. 30
Homework 2: Sept. 6,
Homework 3: Sept. 13,
Homework 4: Sept. 27,
Homework 5: Oct. 4,
Homework 6: Oct. 25,
Homework 7: Nov. 1,
Homework 8: Nov. 8,
Homework 9: Nov. 15,
Homework 10: Nov. 22.

Quizzes:
The purpose of quizzes is to provoke discussion of the course material, and give students feedback on their level of understanding before the exams. Closed book quizzes will be given during the last 20 minutes of four recitations, according to the schedule given in the syllabus. There are no makeup quizzes, but it is to be expected that most students will miss one quiz. Therefore, the lowest of the four quiz scores will be dropped. This is to compensate for illness, bad-thinking days, cars that don't start, etc.

Unless changed by the instructor, 20 minute quizzes will be given during recitation sessions during the weeks of Sept. 9, Oct. 7, Nov. 4, Dec. 2.

Course web page:
The course materials (syllabus, lecture materials, homework assignments, answer keys, etc.) and grades will be uploaded on Carmen (carmen.osu.edu). The instructor will also activate the discussion section of Carmen where you can ask your classmates questions about lecture material, problem sets, etc. To access Carmen, log in with your OSU username (last name.#) and password.

Student responsibility:
Each student receives this syllabus in the first week of the term. It is your responsibility to read this syllabus and be familiar with the course content, procedures, and grading. You are also responsible for any announcements made in class concerning course procedures. (If you are absent, you are expected to get notes, announcements, etc. from another student in the class).

Disability services:
If you anticipate or experience academic barriers based on your disability (including mental health, chronic or temporary medical conditions), please let the instructor know immediately so that we can privately discuss options. To establish reasonable accommodations, the instructor may request that you register with Student Life Disability Services. After registration, make arrangements with the instructor as soon as possible to discuss your accommodations so that they may be implemented in a timely fashion. SLDS contact information: slds.osu.edu; 614-292-3307; 098 Baker Hall, 113 W. 12th Avenue.

Academic integrity:
It is the responsibility of the Committee on Academic Misconduct to investigate or establish procedures for the investigation of all reported cases of student academic misconduct. The term "academic misconduct" includes all forms of student academic misconduct wherever committed; illustrated by, but not limited to, cases of plagiarism and dishonest practices in connection with examinations. Instructors shall report all instances of alleged academic misconduct to the committee (Faculty Rule 3335-5-487). For additional information, see the Code of Student Conduct http://studentlife.osu.edu/csc/.

Diversity:
The Department of Chemistry and Biochemistry promotes a welcoming and inclusive environment for all students and staff, regardless of race, gender, ethnicity, national origin, disability or sexual orientation. There is no tolerance for hateful speech or actions. All violations of this policy should be reported to the OSU Bias Assessment and Response Team (BART, studentaffairs.osu.edu/bias).

The Department encourages diversity at all levels, particularly among the next generation of scientists. Students are encouraged to participate in organizations that provide support specifically for science and engineering students who are African-American, Asian, disabled, Hispanic, LGBTQ or women. These organizations are listed on the Colleges of Arts and Sciences (artsandsciences.osu.edu/stem-organizations) and Engineering (engineering.osu.edu/studentorgs) web sites.