Chemistry 4620, Physical Chemistry II - Spring 2019
Mondays & Wednesdays, 2:15-3:30 pm @ 137 IA (NE)

Main Subjects covered in the course:

○ *Reaction kinetics:*

○ *Introduction to mathematical concepts of quantum mechanics:*
Historical perspective, important mathematical concepts and quantum mechanical postulates, understanding basic machinery to solve a quantum-mechanical problem.

○ *Solutions of Schrodinger equations for basic systems:*
In this part we will focus on solutions relevant to chemistry: particle in the box, harmonic oscillations, 2D and 3D rotations, hydrogen atom, N-electron atoms and molecules.

Lecture textbook:	Ira Levine, Physical Chemistry, 6th edition. It is advisable to get the solutions manual also.
Instructor:	Andrzej Jarzecki, 228NE. tel: 718-951-5000 ext. 2822 e-mail: prof.jarzecki@gmail.com
Office hours:	Mondays & Wednesdays 4:00 pm - 5:00 pm or by appointment.

As you recall the first semester of the course, physical chemistry requires a LOT OF WORK, so make sure you do not have too heavy school schedule and/or other tasks time commitments.

Relevant chapters from the textbook:

Reaction Kinetics. Chapter 16
Quantum Mechanics. Chapter 17
Atomic Structure. Chapter 18
Molecular Electronic Structure, parts of Chapter 19
Molecular Spectroscopy, parts of Chapter 20

Expect additional material relevant for selected topics to be distributed on the lectures or posted on blackboard throughout the semester! Lecture attendance is strongly recommended.

Exams and Tests:

3 midterm exams (100 points each)
1 homework assignment and 1 quiz (60 total points)
final exam, cumulative (200 pts)

A graded homework assignment is going to be more time consuming than those in Chem 4610. The homework assignment (about 8 problems) will be distributed about 2 to 3 week before the due date. Make sure you plan for enough time to complete the assignment.

TOTAL POINT ACCUMULATION IS 760

560 points you earn from the lecture component and it counts for ~74% of your final grade. Additional **200 points** (~26%) you earn from your laboratory component.

Minimum point accumulation to pass the course (D- grade) is 50.5% (**384 points)**

Drop Dates:

February 17 is the last day to DROP a course without a grade.
April 1 is the last day to apply for non-penalty withdrawal (*i.e.,* W grade).

Exam absences:

If you are absent from an exam and have no medical note, your missing grade will be calculated as [(3/4)X + (1/4)Y] – 5 pts, where X and Y are the grades on exams (including the final) closest in time to the missing exam and X < Y. **If you miss two exams without a doctor's note, both exams will be counted as 0.**

You must take the final exam to complete the course.

WEEK 1:

(1) *Jan 27, Mon* – quick review of rates of reactions, rate law from general chemistry

(2) *Jan 29, Wed* – integrated forms of the rate law for zeroth-, first-order reactions

WEEK 2:

(3) *Feb 3, Mon* – second-order reactions, concept of half-life

(4*) Feb 5, Wed* – third-order reactions, half-time, determination of a reaction order

WEEK 3:

(5) *Feb 10, Mon* – parallel and sequential reactions, rate-determining steps, steady-state approximation. **Expect distribution of graded homework assignment** on kinetics (40 pts)

(6) *Feb 19, Wed* – reverse rates and equilibrium reactions

WEEK 4:

(7) *Feb 24, Mon* – mechanism of reactions and rate expressions, methods to measure very fast reactions, relaxation time.

(8) *Feb 26, Wed* – methods to measure very fast reaction (cont.)

WEEK 5:

(9) *March 2, Mon* – methods to measure very fast reaction (cont.),

(10*)* March 4, Wed – **Chapter 17**: historical introduction to concepts of quantum mechanics

WEEK 6:

(11) *March 9, Mon* – **First Midterm Exam**: (Chapter 16: Kinetics) – 100 pts

(12) *March 11, Wed* – basic mathematics for quantum mechanics: Intro

WEEK 7:

(13) *March 16, Mon* - basic mathematics for quantum mechanics
Importance of complex numbers (Euler equations)

(14) *March 18, Wed* - basic mathematics for quantum mechanics
QM postulates, probabilities, commutators

WEEK 8:

(15) *March 23, Mon* – basic mathematics for quantum mechanics
Schrodinger Equation

(16) *March 25, Wed – How does it work?* A quantum particle in the box

WEEK 9:

(17) *March 30, Mon* **– Second Midterm Exam** (Concepts and Mathematics of Quantum Mechanics) – 100 pts
(18) *April 1, Wed* – quantum oscillations; a particle in the harmonic potential

WEEK 10:

(15) *April 6, Mon* – methods for approximate solutions: variational method and perturbation theory
(16) *April 7,* ***Tuesday*** – solutions for 2- and 3-dimentional systems.

WEEK 11:

Other important examples for the exact solutions:
(17) *April 10, Wed* – quantum rotations (in 2 dimensions)
(18) ***April 15, Mon*** – quantum rotations (in 3 dimensions) **SHORT QUIZ (20 pts)**

WEEK 12:

Hydrogen Atom:
(19) *April 20, Mon* – solutions rotations in 3-dimensions for hydrogen atom
(20) *April 22*, *Wed* – Radial part of hydrogen atom and its quantum numbers.

WEEK 13:

(21) ***May 4*, *Mon* – Third Midterm Exam** (Chapter 18: Atomic Structure) – 100 pts
(22) *May 6*, *Wed* – concept of spin, multi-electron atoms, beyond H atom.

WEEK 14:

(23) *May 11*, *Mon* – Born's approximation for electrons in molecules, understanding molecules
(24) *May 13, Wed* - understanding a chemical bonding and molecular spectroscopy.

FINAL EXAM: Wednesday *May 18, 1:00-3:00 pm*