Stony Brook University
Department of Chemistry

CHE 312 – Summer Session I – 2020
Physical Chemistry for the Life Sciences – *Online*
Course Syllabus

CHE 312 - Physical Chemistry for the Life Sciences: (*3 credits*). Provides an understanding of Physical Chemistry concepts to non-chemistry majors, with emphasis on chemical thermodynamics, transport processes, and chemical kinetics.

Prerequisites: CHE 132 or 142; MAT 132 or 142 or 127 or 171 or AMS 161.
Pre- or Corequisite: PHY 121/123 or 125 or 131/133 or 141.

Instructor: Fernando O. Raineri
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Course Objectives:
By the end of the course students will have acquired knowledge on the core aspects of physical chemistry (thermodynamics, electrochemistry, chemical kinetics, quantum mechanics, spectroscopy, and transport processes). More specifically, those students that complete the course will have learned:

1.- the concepts of thermodynamic states, state and path variables, reversible and irreversible processes, and thermodynamic paths.

2.- the laws of thermodynamics, thermodynamic potentials (internal energy, enthalpy, entropy, and Gibbs free energy), and their application to the analysis of chemical reactions and processes relevant to the Life Sciences.

3.- the importance of the chemical potential in applications involving material equilibrium: phase transitions, equilibrium between phases in single and multicomponent systems, chemical equilibrium, and galvanic cells.

4.- how to use rate equations in both differential and integrated form, the role of rate constants in these equations, and their temperature dependence.

5.- the formulation of reaction mechanisms and the concepts and tools required for their analysis: elementary reactions, reaction intermediates, catalysts, rate limiting step, the prior-equilibrium approximation, and the steady-state approximation.

6.- Enzyme catalysis: the Michaelis-Menten mechanism, its quantitative treatment, and the influence of competition and inhibition.

7.- the basic concepts of quantum mechanics: energy quantization, simple systems, and applications in spectroscopy.

8.- the basic ideas of mass transport processes: diffusion and electrical conductivity.

Bibliography:

Physical Chemistry: Principles and Applications in Biological Sciences
I. Tinoco, Jr., K. Sauer, J. C. Wang, J. D. Puglisi, G. Harbison, and D. Rovnyak
5th Edition, Pearson, ISBN-13: 978-0-13-605606-5

Course Information: All course materials will be posted on Blackboard. Every file posting in Blackboard will be followed by an email announcement to the class. More specifically, notes for the contents of every lecture as well as the detailed solutions for the numerical problems will be provided.

Course Details:

The course will consist of the following *online activities*:

(a) ***Recorded lectures, supplementary class notes, and assigned readings.*** The course comprises twelve lectures, each of which covers approximately the materials of three and half normal classes in a semester. These lectures, however, are not offered in synchronous mode. Instead they are posted on Blackboard, under **Documents**, in the form of:

(a.1) Recorded lectures (viewable with a browser). For technical reasons most of the recordings for the lectures can be listened to in the Echo360 link at the top of the Documents folder in Blackboard.

(a.2) Class notes (in pdf format) that explain in detail the material discussed in the recorded lecture. In some cases the notes cover additional materials that, because of time limitations, could not be included in the recordings.

(a.3) The writings (in pdf format) of the recorded lecture.

(b) ***Synchronous recitation and online quizzes on the topics covered in the recitation.*** The recitation (where we discuss selected topics and especially problem-solving) and consultations in the course will be offered in the following online formats:

(b.1) ***Recitation:*** It will be offered in synchronous form on **Monday and Wednesday from 2:00 to 3:30 PM** on Blackboard using Zoom meetings. Exceptions are the days of the midterms and final exam (see below). In these online meetings I will answer any questions from the class (theory or problems). I will also illustrate general approaches to solving problems with carefully selected examples. These meetings give the student the opportunity to clarify concepts or any difficulty that she/he might have with the homework or quiz problems. These recitation meetings **are not** mandatory. The notes of what transpires in these meetings will be posted the same afternoon of the recitation by 5:00 PM. Moreover, the recitations in Zoom will be recorded, and posted in Blackboard (again under the ECHO360 link) the same afternoon of the recitation by 5:00 PM for everyone to access them at any time throughout the course. **Notice: The first recitation will take place on Wednesday, May 27, at 2:00 PM**. *Also please notice that because Memorial Day falls on Monday May 25, the recitation that should have taken place that afternoon will take place (as dictated by the University) on Friday, May 29, at 2:00 PM.* Following that date all classes will follow the Monday-Wednesday Schedule.

(b.2) In addition, students may email me at the email address in the first page, asking any type of questions individually. I will try to answer any question promptly.

(b.3) **Online Quiz every Tuesday and Thursday**. An online quiz, in multiple choice format, will be made available in Blackboard every Tuesday and Thursday from 2:00 PM to 10:00 PM of the following day (Wednesday and Friday). Once the quiz is open, however, the students will have 7 working

hours to complete the solution. Each quiz will focus on problems of the type discussed in the previous day in the recitation. **Notice: The first Quiz will be made available on Thursday, May 28, at 2:00 PM**. *Also please notice that because Memorial Day falls on Monday May 25, the Quiz associated with Class 2 and Recitation 2 will be open on Saturday, May 30, at 2:00 PM and will be due on Sunday May 31 at 10 PM.*

(c) ***Practice problems, with their detailed solutions provided.*** A **Homework** series of problems will be posted the day before each class in Blackboard under **Assignments**. The problems of each Homework will be synchronized with the topics covered in the lectures. The documents posted are as follows:

(c.1) Series of Homework problems (in pdf format). In general these problems *are not* from the end of the chapter in the book (which tend to be long and involved); instead they are relatively short problems that emphasize and supplement the materials treated in the lecture. **These Homework problems are not collected; they are for the student to practice.**

(c.2) Detailed Solutions for the Homework problems (in pdf format). The detailed solutions for each problem in the series are posted one or two days later. This is so that the student can see in detail how problems are solved: how to think about the problem, how to organize and reach the solution, and how to deal with the units.

(d) ***Supplementary end-of-chapter book problems.*** To supplement the Homework problems, a few selected problems from the end of each chapter of the book are considered. These Homework problems are not collected; they are for the student to practice. They are posted on Blackboard, a day or two after each lecture, under **Documents** as follows:

(d.1) Series of Additional Problems from the Book (in pdf format).

(d.2) Detailed solutions for each problem (in pdf format).

Exams: There are two midterm exams, as well as a final exam. **The final exam is not cumulative**. The exams take place on Wednesday, in the time slot 3:30 to 5:30 PM. **There will be no recitation the Wednesday of each exam**. The exams will take place online as Blackboard Assignments, and the specific instructions concerning

them are noted below. *Those students that because of other obligations cannot take the exams at the time indicated above will be offered, on a case by case basis, the possibility of taking the exam during the evening.* The exam dates are as follows:

Exams: (1) Wed. June 3, 3:30 - 5:30 PM.

(2) Wed. June 17, 3:30 - 5:30 PM.

Final: Wed. July 1, 3:30 - 5:30 PM.

If the student has problems with the exam time slot, he/she should contact me (for each of the three exams) to arrange for a special time slot of the corresponding evening.

About the Exams: Please read the following instructions very carefully.

(i) Most of the students are expected to take the midterm and final exams on the respective day from 3:30 PM to 5:30 PM. If for any reason you cannot take the exam during the afternoon hours, please email me indicating (1) the reason and (2) the time that night at which you can take the exam. I expect that everyone that can't take the midterm in the afternoon will take it at night. At night there will be only one time slot, that most likely will go from 9:00 PM to 11:00 PM, eastern time.

(ii) The exam consists of 5 problems for a total of 105 points (you get an A with 90 points or above) and is taken as a Blackboard Assignment. The exam is open book, you don't need to memorize anything. The exam however is not in multiple choice format. **Absolutely every answer that you enter MUST be accompanied with an explanation.** For example, if a question is asking for the final temperature in a process and you calculate the answer to be 300 K, it is NOT ENOUGH to answer the question with the number. *An explanation on how and why you obtained the result must accompany the answer. Even if 300 K is correct, if there is no explanation, the answer is not counted. Also, numerical answers must be accompanied by the appropriate units.*

(iii) In an exam as an assignment you download the exam and solve it at home writing with high contrast ink on clear paper. After you are done (1) you will scan or take photos of your work with your phone, (2) if possible (not absolutely necessary) you will assemble the work as a single pdf file, and (3) you will email it to my email account fernando.raineri@stonybrook.edu no later than 30 minutes after the exam ends.

It is necessary that we do the exams in this way, with an explanation accompanying each answer, so that a partial credit can assigned when the answer is incorrect. Again, anything that you do must be supplemented with an explanation or justification.

Grading

The final grade is calculated as follows:

(a) The two midterms and the final exams count for 27% of the grade each.

(b) The online quizzes count for 19% of the grade.

(c) The letter grades are assigned according to the following cutoffs:

$$\begin{array}{rrr} & \mathrm{A} \geq 90\% & \mathrm{A}- \geq 85\% \\ \mathrm{B}+ \geq 80\% & \mathrm{B} \geq 75\% & \mathrm{B}- \geq 70\% \\ \mathrm{C}+ \geq 65\% & \mathrm{C} \geq 55\% & \\ & \mathrm{D} \geq 45\% & \mathrm{F} < 45\% \end{array}$$

Mathematical Level

We will make liberal use of mathematical results and manipulations to develop theoretical and computational skills to make quantitative predictions. It is assumed that students are comfortable with 1-variable Calculus. A brief extension to calculus of more that one variable will be provided in the class.

Disability Support Services (DSS):

If you have a physical, psychological, medical, or learning disability that may impact your course work, please contact Disability Support Services (631) 632-6748 or http://studentaffairs.stonybrook.edu/dss/. They will determine with you what accommodations are necessary and appropriate. All information and documentation is confidential.

Students who require assistance during emergency evacuation are encouraged to discuss their needs with their professors and Disability Support Services. For procedures and information go to the following website: http://www.stonybrook.edu/ehs/fire/disabilities/asp.

Academic Integrity:

Each student must pursue his or her academic goals honestly and be personally accountable for all submitted work. Representing another person's work as your own is always wrong. Faculty are required to report any suspected instance of academic dishonesty to the Academic Judiciary. For more comprehensive information on academic integrity, including categories of academic dishonesty, please refer to the academic judiciary website at http://www.stonybrook.edu/uaa/academicjudiciary/

Critical Incident Management:

Stony Brook University expects students to respect the rights, privileges, and property of other people. Faculty are required to report to the Office of Judicial Affairs any disruptive behavior that interrupts their ability to teach, compromises the safety of the learning environment, and/or inhibits students' ability to learn.

Summary of Contents

The First Law of Thermodynamics. Systems and surroundings. Energy conversion and energy conservation. Work and Heat. Functions of state. Enthalpy. Phase changes. Thermochemistry. Molecular interpretations of energy and enthalpy.

The second Law of Thermodynamics. Entropy. Entropy changes for spontaneous processes. Molecular interpretation of entropy. Dependence of entropy with temperature at constant pressure. Absolute values of entropy through the Third Law of Thermodynamics. Helmholtz and Gibbs free energies, and their applications.

Free Energy and Chemical Equilibrium. Chemical potential. Ideal and non-ideal gas mixtures. Chemical reactions involving gases. Chemical reactions in solution. Equilibrium constants. Galvanic cells. Standard electrode potentials. The Nernst equation. Biochemical applications of thermodynamics.

Free Energy and Physical Equilibria. Membranes and transport. Ligand binding. Colligative properties. Phase equilibria. One-component systems. Solutions of two or more components. Biological applications.

Rates of Chemical Reactions. The rate law. Order of a reaction. Zero-, first-, and second-order reactions. Elementary steps. Reaction mechanism and the rate law. The steady state approximation. The rate constant and its dependence with temperature. Transition-state theory. Biological applications.

Catalysis. Enzyme kinetics. Catalysts and their effect on reaction rates. Enzyme Catalysis. Michaelis-Menten kinetics. Competition and inhibition. Allosteric effects.

Quantum Mechanics. Wavefunctions. Schrödinger Equation. Particle in a 1-dimensional box. Tunneling. Harmonic Oscillator. Electronic states of molecules.

Spectroscopy. Electromagnetic spectrum. Absorption and Emission of Radiation. Beer-Lambert Law. Fluorescence and Excitation Transfer. Optical Rotatory Dispersion and Circular Dichroism. Nuclear Magnetic Resonance.

Molecular Motion and Transport Properties. Diffusion. Viscosity. Electrophoresis.

Molecular Structures and Interactions. Intermolecular and intramolecular forces. Bond stretching and bond angle bending interactions. Rotation around bonds. Non-covalent interactions. Electrostatic energy. Net atomic charges and dipole moments. Dipole-dipole interactions. London attraction. van der Waals repulsion. London-van der

Waals interaction. The lowest energy conformation. Hydrogen bonds. Hydrophobic and hydrophilic environments.