Chemistry 5400: Biological Physical Chemistry – Winter 2016
(CRN: 21014)

Lectures:	T/Th 4:00-5:50 PM; Room 0025 State Hall
Instructors:	G. Andrés Cisneros; H. Bernhard Schlegel
Office:	333 Chemistry; 375 Chemistry
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Office Hours:	Thursdays 2:00-3:00 PM
Course Website:	http://blackboard.wayne.edu/

Course Objective: Presentation of physical chemistry topics: thermodynamics, solution equilibria, chemical kinetics, quantum chemistry, spectroscopy, statistical mechanics, transport processes, and structure with biological applications.

Student Learning Outcomes: As a result of your studies in Chemistry 5400, Biological Physical Chemistry, you will demonstrate the following abilities:

--- To understand the 3 laws of thermodynamics.
--- To use the 3 laws to derive relationships (equations) between internal energy, free energy, heat, work, and entropy.
--- To differentiate spontaneous from non-spontaneous processes.
--- To apply thermodynamics equations to solve problems involving chemical and physical equilibria of biological molecules including proteins, nucleic acids, carbohydrates, and metabolic intermediates.
--- To understand the statistical foundations that underlie thermodynamics. This includes the Maxwell-Boltzmann distribution, partition functions, and statistical mechanics of entropy.
--- To apply concepts of diffusion and molecular transport theory to random walk processes, centrifugation, protein folding, cooperative binding, viscosity, and gel electrophoresis.
--- To understand the principles of chemical kinetics. To identify the molecularity of a reaction based upon the observed concentration dependence of the rates.
--- To apply the concepts of chemical kinetics to enzymes. To graph rate data in multiple ways (Lineweaver-Burke, Eddie-Hofstee, etc.) to determine the Michaelis constant and the kcat for a reaction.
--- To learn the fundamental concepts of quantum mechanics including the particle in a box, harmonic oscillator, and rigid rotor.
--- To apply those concepts to understand the electron configurations of atoms, molecular orbitals, molecular bonding and structure, and non-covalent interactions.
--- To synthesize a combination of thermodynamics, quantum chemistry, molecular structure, and non-covalent interactions to understand the protein folding problem.
--- To apply classical molecular dynamics simulations to biological macromolecules.
--- To apply quantum mechanics principles to understand optical spectroscopies including UV, IR, fluorescence, and circular dichroism.
--- To understand the theory of X-ray diffraction of macromolecules. This includes the crystal symmetry, scattering of X-rays by periodic electron density, Miller indexes, understanding the Phase problem, interpreting the diffraction pattern in reciprocal space and real space, and refinement. Understanding how the resolution and R-factor affect the quality of the electron density using a Luzzati plot.

Prerequisite: Prereq: a grade of C or above in CHM 2280 or equiv.; MAT 2020 or equiv.; prereq. or coreq: MAT 2030, PHY 2170, or equiv.

Textbook: Physical Chemistry: Principles and Applications in Biological Sciences – 5th Edition, Tinoco, Sauer, Wang, Puglisi, Harbison, and Roynyak, Pearson 2014.

Optional Book: Understanding Thermodynamics, H.C. Van Ness, Dover, 1983. $8.00 on Amazon – very helpful book for students.

Grading:

	5 Homeworks	(>80% completed)	50 pts
	5 Quizzes (lowest quiz dropped)	(5 x 10 pts)	50 pts
	2 In class Exams	(3 x 150 pts)	200 pts
	Cumulative Final Exam		200 pts
	total		500 pts

Homeworks: There will be homeworks offered every week throughout the semester.

Quizzes: There will be six Quizzes offered throughout the semester. Each Quiz will be worth 10 pts. There are no makeup quizzes for any reason. The lowest quiz will be dropped. Quiz dates will not be announced ahead of time, so you need to be prepared throughout the course since a quiz could be given at any class session.

Exams: There will be 2 mid-term exams and a comprehensive final exam. Final exam conflicts should be rectified with the instructor in advance. There will be no makeup exams.

Class Sessions: Lectures will be used to clarify and work with important topics. You are expected to be prepared on the material to be discussed when you come to class. The best way to prepare is to read the corresponding chapter ahead of class.

Attendance: Attendance at all class sessions is required. Absence from classes where a quiz or exam is given will result in a zero grade for the quiz or exam offered on that day.

Grading Scale: The typical grading scheme is as follows, but deviations from this scale may be seen from year to year**. We reserve the right to rescale the final grades** if this scale proves unsatisfactory. Posting of grades: The final course grades will be posted on Pipeline, whereas individual test scores will be posted on Blackboard.

Final Overall Average (%)	Final Course Grade	Final Overall Average (%)	Final Course Grade
93 - 100	A	70 – 73	C
88 – 92	A-	67 – 70	C-
83 – 88	B+	63 – 67	D+
80 – 83	B	60 – 63	D
77 – 80	B-	57 – 60	D-
73 – 77	C+	below 57	F

*Please note that students who withdraw after the 4th week will receive a WP, WF, or WN grade.

Registration and Withdrawals: All students must be formally registered in this course before the first exam. Withdrawals up to February 8, 2015 will not appear on your record. No withdrawals will be approved after **March 29, 2015**.

Lectures: The lectures will be used to present and clarify important topics, including material from the text. It is important to take precise and understandable lecture notes. If a class is missed, it is your responsibility to obtain the missed lecture notes and other materials, handouts and announcements (e.g., exam date changes, etc.) from Blackboard or classmates. **Reading/Skimming the Chapters before the lectures is highly advised**. This will help you to get more out of the lectures. Note: some topics will be covered that are not in your textbook; therefore, it is essential to attend the lectures. **The emphasis on exams will be material covered in class and presented on lecture slides.**

Lecture Recordings: Both the Audio and video of Lectures are captured. You can download the movie files by going to Blackboard and clicking on the "EchoCenter" link on the left panel.

Office Hours: Office Hours will be on Thursdays 2:00-3:00 PM. Those who cannot make these hours should make an appointment by email to either instructor for other times.

Academic Integrity: For all examinations, you may not leave the classroom in the middle of the exam and then return to continue with the examination. If there are any questions or concerns regarding the grade for any examination, these questions can be brought to attention of Dr. Cisneros or Dr. Schlegel no later than ONE week after the graded exam is returned. Any dishonest behavior is dealt with in accordance with the university policies on cheating. To avoid the potential for dishonesty, such as individuals who make changes in their graded exams and then request regrading, the graded exams are routinely photocopied before they are returned. Any examination turned in for regrading will be compared against the photocopy, therefore please do not write on the examination paper after it is graded if you intend to request regarding.

Cheating: Cheating on examinations/quizzes or any other sort of dishonesty are abhorrent to the academic process. Cheating shall result in severe punishment, and may lead to expulsion from the University, following the rule of the College of Liberal Arts and Sciences and the University. The usual punishment for cases of cheating (first offense) in this course are (a) expulsion from the course with a grade of "F" and (b) a recommendation to the Dean of the College that the incident be recorded in the permanent record of the student for 4 years, or until the date of the student's graduation, whichever comes first. All work needs to be independent and not copied from another student or any other source.

Special Help and Problems: Students with special problems or any questions concerning the course should consult with the instructor as soon as possible:

STUDENT DISABILITY SERVICES: If you have a documented disability that requires accommodations, you will need to register with Student Disability Services for coordination of your academic accommodations. The Student Disability Services (SDS) office is located at 1600 David Adamany Undergraduate Library in the Student Academic Success Services department. The SDS telephone number is 313-577-1851 or 313-577-3365 (TDD only). Once you have your accommodations in place, I will be glad to meet with you privately during office hours to discuss your special needs. Student Disability Services' mission is to assist the university in creating an accessible community where students with disabilities have an equal opportunity to fully participate in their educational experience at Wayne State University.

Social Media Policies: Please see the document on the Blackboard site for this course (under "content")

WSU Resources for Students
Student Disability Services (SDS) http://studentdisability.wayne.edu/
Academic Success Center http://www.success.wayne.edu/
Counseling and Psychological Services (CAPS) http://www.caps.wayne.edu
Dean of Students' Office http://www.doso.wayne.edu
College of Liberal Arts & Sciences: http://clasweb.clas.wayne.edu/CurrentStudents

Succeeding in this course:

- Stay on top of the material. This course requires A LOT of reading, thinking and processing.
- Read assigned reading before coming to class. You will get more out of each lecture this way.
- Ask questions and participate in the class exercises (group and individual).
- Study in groups. Bouncing ideas off of your peers is a great way to fix information in your mind. Explaining ideas to others is a great way to make sure that you understand the material yourself.
- Don't cram for exams. A lot of the material in this course builds upon basic comprehension of earlier lectures. Cramming will not work!
- Come to my office hours!

Tentative Class Schedule for CHM5400 (Winter 2015)*

Date	Day	Class	Topic	Reading	Homework|Quiz Due	
Jan. 12	T	1	Course Introduction, Structure of Biomolecules	**Ch 1**		1/12
Jan. 14	Th	2	First Law of Thermodynamics	**Ch 2**		
Jan. 19	T	3	First Law of Thermodynamics	**Ch 2**		
Jan. 21	Th	4	Second Law of Thermodynamics	**Ch 3**	1/21	1/21
Jan. 25			Last Day to drop with 100% Tuition cancellation			
Jan. 26	T	5	Second Law of Thermodynamics	**Ch 3**		
Jan. 28	Th	6	Free Energy and Chemical Equilibria	**Ch 4**	1/28	
Feb. 2	T	7	Free Energy and Chemical Equilibria	**Ch 4**		
Feb. 4	Th	8	Statistical Foundations of Biophysical Chemistry	**Ch 5**	2/4	2/4
Feb. 7			Last Day to drop with no grade reported (no refund)			
Feb. 9	T	9	Statistical Foundations of Biophysical Chemistry	**Ch 5**	2/9	
Feb. 11	Th	10	**Exam 1 (Lectures 1-9)**			
Feb. 16	T	11	Early Assessment of Course Grade			
Feb. 16	T	11	Physical Equilibria	**Ch 6**		
Feb. 18	Th	12	Physical Equilibria	**Ch 6**	2/18	2/18
Feb. 23	T	13	Motions of biological Molecules	**Ch 8**		
Feb. 25	Th	14	Motions of biological Molecules	**Ch 8**	2/25	
Mar. 1	T	15	Kinetics: Rates of Chemical Reactions	**Ch 9**		
Mar. 3	Th	16	Kinetics: Rates of Chemical Reactions	**Ch 9**	3/1	3/1
Mar. 8	T	17	Enzyme Kinetics	**Ch 10**		
Mar. 10	Th	18	Enzyme Kinetics	**Ch 10**	3/10	
Mar. 15	T		No Class – Spring Break			
Mar. 17	Th		No Class – Spring Break			
Mar. 22	T	19	Quantum Mechanics	**Ch 11**	3/22	
Mar. 24	Th	20	**Exam 2 (Lectures 10-18)**			
Mar. 27			**Last day to withdraw (instructor approval required)**			
Mar. 29	T	21	Quantum Mechanics	**Ch 11**		
Mar. 31	Th	22	Quantum Mechanics	**Ch 11**	3/31	3/31
Apr. 5	T	23	Non-covalent interactions	**Ch 12**		
Apr. 7	Th	24	Molecular Dynamics simulations	**Ch 12**	4/7	
Apr. 12	T	25	Optical Spectroscopy	**Ch 13**		
Apr. 14	Th	26	Optical Spectroscopy	**Ch 13**	4/14	4/14
Apr. 19	T	27	X-ray Crystallography of biomolecules	**Ch 15**		
Apr. 21	Th	28	X-ray Crystallography of biomolecules	**Ch 15**	4/21	
Apr. 26	T		Study Day			
Apr. 28	Th		**Final Exam (Cumulative) – normal time and place**			

*** Note that lecture schedule is tentative and likely will be changed throughout the semester**