Physical Biochemistry
Course Syllabus

BCHM 485: TuTh, 9:30-10:45am, CHEM 2201 (before the spring break)
and online after March 30
Spring 2020

Professor: David Fushman
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e-mail: **fushman@umd.edu** (much preferred to phone). Please restrict telephone inquiries to office-hour times, except in "emergencies". Email is welcome anytime.
Office hours: Tuesday, 12:30-2:30 pm

Teaching Assistant/Grader: Andrew Boughton, Office hours**:** Thursday, 2-4 pm, Room 1106 Biomolecular Sciences Bldg (#296), voice: x55474, e-mail: ajb210@umd.edu

Course Description

This is part II of the Physical Chemistry course designed to cover topics of particular relevance to problems and applications of physical methods to modern biochemistry. In addition to covering the principles and applications of quantum mechanics and statistical thermodynamics there is emphasis on various experimental techniques: sedimentation, chromatography, electrophoresis, a broad range of spectroscopies and their applications to biomacromolecules, and on methods for biomolecular structure determination.

Mathematical level required. Physical chemistry is a rigorous quantitative discipline. Many of the problems and methods discussed throughout the course require familiarity with the following mathematical techniques: logarithms and exponentials, trigonometric functions, complex numbers and complex functions, basic vector analysis, matrix algebra (including determinants and eigenvalue equations), differential and integral calculus, power series and Taylor expansion, ordinary and partial differential equations.

Textbooks:

Required:

(1) Thomas Engel, **Quantum Chemistry & Spectroscopy,** 3rd edition, Pearson, Benjamin-Cummings Pub Co.
(2) Thomas Engel & Philip Reid, **Thermodynamics, Statistical Thermodynamics, and Kinetics,** Pearson, Benjamin-Cummings Pub Co. (3rd edition). The **Molecular Thermodynamics** textbook by McQuarrie & Simon that you might have from the CHEM481 course could be sufficient.

Additional recommended sources:

(1) Peter Atkins, Julio de Paula, *Physical Chemistry*, 8th edition; Either complete book or *Volume 2: Quantum Chemistry, Spectroscopy, and Statistical Thermodynamics*, W. H. Freeman & Co, New York
(2) David Eisenberg, Donald Crothers, *Physical Chemistry with Applications to the Life Sciences*. Benjamin/Cummings Publishing Co.
(3) Dill & Bromberg *Molecular Driving Forces.*

(4) Cantor & Schimmel *Biophysical Chemistry*.

There is a course homepage at:

http://terpconnect.umd.edu/~fushman/

where you will find a copy of the syllabus, regular homework and reading assignments, exam solutions and statistics, and extra material. Some of these materials will be posted as we proceed with the course. You are welcome to email me your questions and comments. I do not guarantee individual responses, but errors or common points of confusion will be addressed in class and/or in the Q&A section of the website. Links to course pages from previous years can be found at **http://gandalf.umd.edu/FushmanLab/**

Class format. ***Lecture attendance is important and expected.*** The lectures will not replace the textbook but rather supplement it with new material, emphasize important conceptual and technical issues, and clarify tricky points. You are responsible for both the material covered in the lectures and the assigned reading. **Please ask questions in lecture if something is not clear!**

If you believe a mistake has been made in lecture (it's likely to happen), please speak up or inform me afterward.

IMPORTANT Changes After March 30: As we transitioned to online education during these difficult times, the lectures will be delivered asynchronously. They will be recorded and made available via ELMS on Tue/Thu, the same days that were originally reserved for in-class lectures. In addition to the video recording, I will also upload a PDF copy of the lecture. Office hours will be held online via zoom on Tuesdays 12:30-2:30 pm. I will email you zoom meeting information. If you can't connect during this time but want to speak with me, I will be happy to arrange a zoom meeting at a different day/time. My goal is to accommodate as many of your requests as possible. If there is high demand for zoom interactions, I can try holding office hours during the "original" lecture time.

The remaining two graded homeworks and the exams will be given via ELMS.

Examinations will be given on the following dates:

Exam I:	Tuesday, March 10
Exam II:	Thursday, April 23 (tentative)
Final exam:	**Friday, May 15 (**This exam date is firm, for now)

Midterm exams will include only the material covered since the previous exam but will inevitably draw on information from earlier in the semester. The final exam will cover the entire course material. The exams will include material covered in the lectures and in the corresponding sections of the textbooks. You will be allowed to use calculators on the exams for computations only.

Homework. Questions and problems will be given as homework regularly: they are designed to encourage your regular reading of the material, and completing them will help you prepare for the exams. In addition, ***graded homework problems*** will be handed out regularly. You are expected to hand in the worked problems before or on the day the problem set is due.

Grading Policy.

Midterm exams ……………..….	100 points each
Graded homework …...…….	100 points total
Final exam …………………..	100 points

Your final letter grade will be based on your total score on the two mid-term exams, the final exam, and the graded homework problems (**maximum = 400 points**). Grading will be done on a *curve* based on the overall distribution of the *class scores*. You will be guaranteed an A if your total score is above 85% of the class, a B if it is above 60% of the class, and a C if it is above 30% of the class scores. In addition, students who scored ≥ 340 points (i.e. ≥ 85% of max score) will be guaranteed an A, and those with ≥ 180 points (i.e. ≥ 45% of max score) will be guaranteed a passing grade (C or higher), *independent of the curve*. After the cut-offs for A, B, etc grades are determined, the final grading will be done using the "+/–" grading system.

Re-grades. If you think a mistake has been made in grading your work, you *must* submit it to me for re-grading no later than one week after the date on which the work was returned to the class, with a written explanation of your reasons for desiring a re-grade. The entire exam is subject to re-grading, which often decreases the total score. After that, the grade will be considered final. Arithmetic errors in the grading can be corrected without re-grading.

Make-up exam policy. ***Do not miss any of the exams or graded homework problems***. If you miss an exam, **you will have a score of "0" on the exam until it is made up.** Only students with **legitimate excuses** as determined by the University policy will be given a make-up exam. For a make-up exam you will need a written documentation of the emergency or illness. A missed or late homework will be assigned a score of "**0**"**; there will be no make-up for homework problems.**

It is your responsibility to contact me promptly to schedule a make-up exam. In any case, YOU MUST CONTACT ME WITHIN 24 HOURS OF MISSING AN EXAM.

All students must take the final exam.

Please notify me as soon as possible if you know ahead of time that you will miss an exam for any reason, including previously scheduled events, religious observances, etc. According to the University policy you must tell me no later than February 7 (the last day of schedule adjustment for Spring 2020).

Teaching assistance. There will be no teaching assistant for this course because the Department did not provide us with a TA position. *Andrew Boughton*, an advanced graduate student in the Biochemistry program, will help me grade the exams and some graded homeworks. I will be happy to help you with the material during my office hours. If necessary, I will try to arrange other times to meet.

The University course-related policies can be found at:
http://www.ugst.umd.edu/courserelatedpolicies.html .

Academic integrity. Students are expected to observe the University's *Code of*

Academic Integrity (**http://shc.umd.edu/SHC/Default.aspx, http://www.president.umd.edu/policies/iii100a.html**). Students are responsible for knowing, understanding and behave accordingly to the content of the Code. Cheating on the exams or problem sets is not acceptable and will be met with zero tolerance. Specific guidelines relevant to this course include:

1. All work that you submit for grading in this course must be the original work of the student whose name is on the work.
2. You may use a **standalone** calculator (**not** on your **Smartphone!**) for the exams, but **only** for computation. Any other use is a violation of the University's *Code of Academic Integrity*.
3. Other actions such as falsification of excuses for missed exams or submission of an altered, graded examination for re-grading, etc., are violations of the *Code of Academic Integrity* or the *Code of Student Conduct.*

Honor Pledge. Students will be required to write and sign on the front cover of each exam the Honor Pledge: "I pledge on my honor that I have not given or received any unauthorized assistance on this examination". More information on the Honor Pledge can be found on the University website **http://www.ugst.umd.edu/courserelatedpolicies.html**.

Religious observance. It is the student's responsibility to inform me in advance of any intended absences for religious observances. Notice should be provided as soon as possible but no later than the end of the schedule adjustment period (February 7th).

Students with disabilities. If you have a documented disability and wish to discuss academic accommodations with me, please contact me as soon as possible.

Course Outline

The exact order of topics and the number of lectures on each may change.

1. Quantum Mechanics. (5.5 weeks)
Postulates of quantum mechanics. Observables and operators, wave functions and eigenvalues, the uncertainty principle, Schrödinger's equation. Quantization of energy, a particle in a box, harmonic oscillator. Quantization of the angular momentum, rotation in two and three dimensions. Hydrogen atom. Electron spin, Pauli principle. Atomic orbitals. Molecular structure, rotation and vibration, Born-Oppenheimer approximation.

2. Spectroscopy. (2 weeks)
Transitions and selection rules. Vibrational and rotational transitions. Electronic transitions. Optical spectroscopy. Applications to biomolecules: absorption, circular dichroism, fluorescence techniques. Magnetic resonance spectroscopy, applications to biomolecular structure and interactions.

3. Statistical thermodynamics. (3 weeks).
Configurations, micro- and macrostates. The Boltzmann distribution. The concept of partition function. The concept of ensemble. From partition function to thermodynamic functions. Applications to binding equilibria, single- and multicomponent systems, phase transitions. Statistical mechanics of biomolecules as polymer chains. Helix-coil transition, protein folding.

4. Molecular motion. (1.5 weeks)
Kinetic theory of gases. Maxwell-Boltzmann. Transport phenomena, Fick's laws, diffusion equation. Applications to biochemistry: dialysis, liquid chromatography, sedimentation, electrophoresis.

5. Chemical and biochemical kinetics. (1.5 weeks)
General kinetics. Differential and integrated rate laws. Mechanisms of chemical and biochemical reactions, enzyme kinetics. Transition state theory. Diffusion-limited processes. Kinetics methods in biochemistry.