Physical Biochemistry
Course Syllabus
Spring 2022
BCHM 485: TuTh, 9:30-10:45am, CHEM 1402

Professor: David Fushman
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Office hours: Thursday, 4:30-6 pm via zoom: **https://umd.zoom.us/j/8653743671**

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Office hours**:** Tuesday, 5-6 pm via zoom: **https://umd.zoom.us/s/3826284634**

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: a broad range of spectroscopies and their applications to (bio)molecules, and on methods for biomolecular structure characterization, as well as sedimentation, chromatography, and electrophoresis.

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 Atkins' textbook 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 lectures and the assigned reading. **Please ask questions in lecture if something is not clear!**

You must fully comply with the COVID-19 related campus policies and rules for in-person teaching. There will be zero tolerance for any violations of these policies and rules. If we transition to online education, lectures will be delivered synchronously (via zoom) or asynchronously (as prerecorded videos). They will be recorded (using zoom) and made available via ELMS.

Office hours will be held online via zoom. If you can't connect during the allocated time but want to speak with me, I will be happy to arrange a zoom meeting at a different day/time. Our goal is to accommodate as many of your requests as possible. If there is high demand for zoom interactions, we can try holding office hours during the "original" lecture time.

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

Examinations will be given on the following dates:

Exam I:	Tuesday, March 15 (tentative)
Exam II:	Thursday, April 28 (tentative)
Final exam:	**Friday, May 13, 8:00-10:00 am (**This exam date is firm)

Midterm exams will include only the material covered since the previous exam but will inevitably draw on the information from earlier in the semester. 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 end-of-chapter 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 will have to submit your answers to the graded homework problems via ELMS by the specified deadline.

Grading Policy.

Midterm exams ………………	100 points each
Graded homeworks ……..……	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 the max score) will be guaranteed an A, and those with ≥ 180 points (i.e. ≥ 45% of the 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 will be subject to re-grading, which could decrease 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 graded homework will be assigned a score of "**0**".

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.

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 4th (the last day of schedule adjustment for Spring 2022).

Teaching assistance. There will be no teaching assistant for this course because the Department did not provide us with a TA position. *Raquel Gama Lima Costa*, a graduate student in the Chemical Physics program, will help me grade the exams and graded homeworks. We will be happy to help you with the material during our office hours. If necessary, we 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 4^{th}).

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. (7.5 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. Many-electron atoms, atomic orbitals, electron spin, Pauli principle. Molecular structure, quantum-mechanical nature of a chemical bond, Born-Oppenheimer approximation, molecular rotation and vibration.

2. Spectroscopy. (2.5 weeks)
Transitions and selection rules: a quantum-mechanical treatment. 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. (2.5 weeks).
Configurations and probabilities, 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 biomacromolecules as polymer chains. Helix-coil transition, protein folding.

4. Molecular motion. (1 week)
Kinetic theory of gases. Maxwell-Boltzmann. Transport phenomena, Fick's laws, diffusion equation. Applications to biochemistry: dialysis, liquid chromatography, sedimentation, electrophoresis.