General Information and Syllabus

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Moodle: All material associated with this class will be posted on the Moodle homepage at moodle.haverford.edu. The instructor will make you an enrolled student to this page after the first class meeting if you are not preregistered.

Office hours: By appointment and listed weekly on Moodle for both the instructor and the TA. (Please provide feedback about the timing of office hours!) Office hours will be generally designed for students to work together with TA or instructor support; please make appointments for one:one meetings with the instructor.

Class: Tuesday and Thursday from 8:35 to 9:55 a.m., Room E309, KINSC.

It is possible that I will be out of town for the regular class on Tuesday, Apr. 2: for that week I tentatively propose to "make up" that class on Sat., Apr. 6 at 9:00-10:30 am, pending unanimous class availability.

Snow days: if the College closes and classes are cancelled during the regular meeting time for this class, the class will not be made up and students are responsible for completing the posted in-class problems (which might be adjusted based on class cancellation). In most such cases, the instructor will be present in the classroom at the regular class time to assist with problems.

Prerequisites: Math 121 or 216. We will use matrix manipulation techniques extensively, but Math 215 is not required. There are math resources that either appear in the textbook or will be posted on particular topics (including matrices and linear algebra) throughout the course. Please let the instructor know if you have not taken Chem 111 or an equivalent course that covers bonds, molecular orbitals, and basic structural organic chemistry.

The McQuarrie text is the main textbook for this course. The Engel text offers an e-version that can be purchased for less than the hardcover version, and some students find its treatment of some topics more immediately accessible. It also treats a few topics much more thoroughly than the McQuarrie book. Absolutely required sections and problems from the Engel book will be posted on Moodle during spring 2019.
Required: Joshua Schrier, *Introduction to Computational Physical Chemistry* (University Science Books, 2017). We will use approximately half of this book, which is also available from the publisher as an e-book: purchasing "lifetime access" is recommended because this book is also used in Chem 304.
Grades: Grades will be calculated on the following basis:
5% pre-class questionnaires (see below)
5% attendance and in-class participation (see below)
5% weekly written journal entries (see below)
20% submitted problems (see below)
20% midterm exam #1 (see below)
20% midterm exam #2 (see below)
25% comprehensive final exam

Attendance: Attendance at all class sessions is a requirement of this course. Your physical presence is necessary, but not sufficient. Be prepared to interact with your classmates, discuss the material, and do problems together, since most classes will consist of no lecture material and mainly of activities and problems with some discussion. Any planned absence (i.e. for athletic events or other special circumstances) must be discussed with the instructor as early as possible in the semester.

Problem Sets: The only way to understand quantum mechanics is to (1) do problems, and (2) to communicate with other people about what is bugging you or where you are stuck. Chemistry in general is a “doing” discipline as much as a conceptual discipline and that especially holds for its most quantitative and fundamental pieces, which you will encounter directly in this course. All problem set due dates will be posted on Moodle; in general problem sets will be due on Monday morning of the week following when problems were assigned and worked in class. You will electronically submit all of the problems from the previous week. You should keep a copy of all completed problems in your own notes, since these will form a central part of your own notes for the exams and future pieces of the course; this copy will also allow you to generate a revised version of any problem if you desire more credit. After the first submission and grading, problems may be revised for more credit up until each exam. Please write each problem on its own page for ease of submission and record-keeping. Please clearly annotate each problem so it is clear to you what you actually solved or showed in the problem: solely showing algebra and/or equations provides an insufficient answer to most problems in this course.

Exams: All exams are open-book, open-notes, open-Moodle, open-Mathematica, etc., but you are not allowed to consult any resources outside of this course (meaning, no other people and no net-searching). After downloading the test file, you will have one contiguous 24 hour period to complete each midterm exam. The exam problems will be practically simpler than many problem set questions in the level of work required to solve them. Test dates are not set in stone, but here is a draft of the availability windows for the two midterm exams:
Feb. 28-Mar. 5
Apr. 4-Apr. 9 (subject to change)
The material for each exam will be clearly advertised in advance of each exam. Since this course is very much a building-up process, the second midterm may contain material from the first part of the course. The final exam is open-book, open-notes, and comprehensive without any particular weighting towards the end of the course. The final will also be a 24 hour self-scheduled exam.
Software, computers, calculators, and electronic tools:

This is a quantitative course and will deal in both actual numbers (and their units) and variables that change with respect to others in molecular systems. You should always have something that acts easily as a scientific calculator on hand: this could be a handheld calculator, an app on your phone, or the built-in calculator on your computer. Wolfram Alpha can be quite helpful for doing unit conversions when necessary, but you need to make sure that you know what you’re asking it to do for you.

Much of the material in this course is best illustrated and worked through with the help of computational software, and being able to use software to manipulate and visualize models and data is a central part of the current discipline of physical chemistry. We will present many results using Mathematica, and building a strong working familiarity with Mathematica will be a great help to you in this course. Many assignments, including exam problems, will require symbolic or numerical evaluation, graphical analysis or presentation, or both, and Mathematica is well-suited to both kinds of tasks. This software is available for download on the IITS website as linked from the course Moodle page. Other graphics or plotting software may be used in some cases (i.e. spreadsheet programs like Excel or Origin), but the use of Mathematica is strongly encouraged. The course Moodle site includes some links to introduce Mathematica, and I will also post some of the examples that I use in class. The best way to become familiar with Mathematica is frequent and regular use, which we will certainly do in class together but which you should also do on your own to make sure that your skill set is reproducible when in a room by yourself.

You are essentially required to use Mathematica for some class activities, but remember: Mathematica is not a black box. If you use it that way, you will often get nonsense out, so make sure that you understand your specific goals in interacting with Mathematica. Most of the derivations in the main textbook, in particular, can be done more quickly with pen, paper, your brain, and a book of integral tables than with Mathematica. For this reason, I recommend that you have access to a set of Mathematical Tables. The CRC Handbook has these (and I will link to the online version of the CRC), as do the backs of many calculus textbooks that you might own from previous courses. These will make it easy for you to look up derivatives, integrals, series expansions, etc. that you may need in the course of working out homework problems without letting software make your life more difficult. Relying on Mathematica to do integrals and derivatives for you can be a recipe for unnecessary headaches. However, letting Mathematica solve systems of simultaneous equations or keep track of matrix elements can be a lifesaver and enable some much more extensive calculations than you might ever want to do by hand.

Disabilities: Haverford College is committed to supporting the learning process for all students. Please contact me as soon as possible if you are having difficulties in the course, or if you anticipated a disability-related issue. There are also many resources on campus available to you as a student, including the Office of Academic Resources (https://www.haverford.edu/oar/) and the Office of Access and Disability Services (https://www.haverford.edu/access-and-disability-services/). If you think you may need accommodations because of a disability, you should contact Access and Disability Services at hc-ads@haverford.edu. If you have already been approved to
receive academic accommodations and would like to request accommodations in this course because of a disability, please meet with me privately at the beginning of the semester (ideally within the first two weeks) with your verification letter.

**Copyright:** All published material associated with this course is the property of the stated copyright holder and may not be reproduced or reposted outside of the student’s own individual domain without the copyright holder’s explicit permission. Any nonlabeled course materials generated by the instructor are his own intellectual property and may not be reproduced or reposted outside of this course without the instructor’s explicit written permission. Violation of the instructor’s or textbook authors’ intellectual property would constitute an Honor Code violation.

**Honor Code:** The Haverford College Honor Code, as outlined in the Haverford College Catalog and administered by the Honor Council, applies to all submitted work in CHEM 305b. Students will work together on problem sets in class and are encouraged to do so outside of class. It is a requirement of the Honor Code for this course that you note outside of class collaborators on each submitted problem. It is also a requirement that all submitted material be your own; this includes plots and graphics generated using a computer, and especially Mathematica notebooks and plots. You must acknowledge in writing any assistance you receive from literature outside the course materials, other students, non-course textbooks, the internet, or any source but Prof. Londergan.
Preparation: **Readings from the text, other text or online materials, computational demos, and/or lecture videos** will be assigned before each class; it is paramount that you get through all assigned material before each class, since I will assume that you have done so and for all classes you will need to answer online questions on the pre-class material. When questions on the reading are assigned (before every class), they will generally be due **at 10:00pm the night before class**, at which time the submission link on Moodle will become unavailable and your ability to get credit for this assignment will expire. Group activities, problems, and anything else that happens during class will be based on the assumption that you have seen and interacted with all pre-class material, including the videos that will take the place of any in-class lectures.

**Problems** will be assigned for each class as well. (1) There will usually be a few short problems that you must have completed before class: students may be randomly selected at the beginning of class to present problems for that class. (2) Then there will be a set of more extensive problems for us to work on together in class. Please have a preliminary look at these problems and think about them, without necessarily going deep into solving them, before class starts because they will usually be the main subject of our in-class work.

Consolidation: **Writing** (in clear written English, with some inclusion of equations and mathematical expressions) is a central and important part of this course, and it is especially important for helping you to consolidate what you have learned into a form that helps you on exams. As stated above, all submitted problems should be clearly annotated so that the context and point of the problem are clear to any observer (especially you after several weeks).

**Weekly journal entries** are a required part of this course: these will be submitted on Moodle in response to relatively broad prompts at the end of each week, to provide you an opportunity to reflect on that week’s material and express your own understanding (or arguments, or issues) in writing. I will briefly look at these and grade them only for completion, and these entries will not be shared between students. Thornier issues that you would like to discuss with the class can be shared either in class or on the class Piazza page, which has more flexibility than a Moodle forum for keeping track of multiple discussion threads and for posting attached files (i.e. Mathematica notebooks, etc.).
Here is a **recommended strategy** for class preparation, record-keeping, and having yourself ready to take open-book exams:

**Before class:**

1. Read the assigned text material, keeping a running list of the things that you don’t understand, even after you have gone back and thought it over. Do any problems that are assigned to be done before class and be ready to present them if called upon.
2. Watch the video(s) and play with any demo materials, taking your own notes and noting any additional questions that you might have. Videos are not designed to provide comprehensive lecture-style coverage of the text, rather they are designed to point out specific items of interest, emphasize important ideas, and to provide a language basis for what we will do together in class.
3. Answer the online pre-class questions.

**In class:**

4. Be there! Bring your software-enabled laptop and calculator. Present problems as needed.
5. Work on the day’s problems, using your classmates and me as resources and noting the key issues and steps to help you formulate your own solution to the problems.

**After class (i.e., the same day or within one day):**

6. Revise and consolidate your notes on pre-class and in-class material based on what you learned in class. Make sure that you answered your own questions from before class. **Write down important key ideas and equations, and be ready to add those to your weekly journal entry on Moodle.** Having a short, consolidated version of your notes is very important to success on open-book exams.
7. Write down complete, well-annotated versions of the solutions to the problems for your own records. Make sure that they are fully legible when reproduced/scanned/photographed so you can submit them. You might finish these problems or come to your best solution during shared office hours with either the instructor or TA.

**A general note on quantum mechanics and this course:**

“Physical” chemistry consists of observations of the physical behavior of chemical systems and the models which are used to explain and predict this behavior. The goal of this class is learn the models (mental frameworks) and tools (generally mathematical) that will enable you to think and act like a physical chemist. To succeed, you must combine broad knowledge of physical laws and basic quantum mechanical postulates, practical (often rather than particularly elegant) mathematical and computational skill to weave these together, and an intuitive “horse sense” about chemical systems (which can sometimes be contradicted by the results of quantum mechanics, so be ready for that). Unlike physicists, who are interested in “the world as it should be” (i.e., according to a specific model), we are interested in “the world as it is”. Since the world is a complex place, this requires a certain “dirtyness” of our approach, with recourse to experimental parameters, semi-empirical models, etc. and a constant flexibility in thinking about problems from the perspective of models with different levels of “realism”. With that flexibility and a developed toolbox of models and quantitative adjustment techniques (“duct tape”), you can begin to understand and predict the properties of a broad range of chemical systems. One particularly “nice”
thing about this particular course is that there is a clear set of rules that ultimately define how everything in chemistry works, and we will learn them, use them, and also learn how to deal with approximate versions when the “real” rules are either monstrously difficult or impossible to apply to practical situations.

Ultimately, the goal of this course is to develop rigorous definitions of physical properties and the relationships between different physical properties. The best way we have found for organizing logical relationships is mathematics. That being said, this is really not a math course, although at times it’s really going to seem that way. When working with models, please focus on the physical “meaning” of the variables and the relationships that these describe, however crazy those meanings might be (and they are pretty crazy sometimes in quantum mechanics). If you just try to manipulate symbols, without understanding the physical reality that they describe, it will usually just lead to nonsense. Since the models of physical chemistry are mathematical, a large part of learning physical chemistry is learning to use the mathematical language that frames these models, and pieces of this will be re-introduced and introduced as needed for particular kinds of problems.

And: units are very important! and provide an actual connection to the real world, so don’t lose track of them (even in cases where we present problems in some set of “natural” or “reduced” units.

Advice from previous students:

"Even though you think you don't need to, make a table-of-contents for McQuarrie as you go along. It really helps to have it written down where the table with all the ground-state configurations, or whatever, is exactly."

"Take careful notes on the videos and go to TA sessions."

"Check the pre-class questionnaire before you do the readings, so that you know what minutiae are important to pick out. Lean on your fellow students when you don't understand something."

"Do the practice exams and get help with them before tests because the actual exams have very similar questions. Also figure out what resource works best for you and dedicate the majority of the time to that one then skim the others if you don't have time to do everything in a lot of depth."

"Try to get as much done as possible in class and find a good team of people to work on problems with because you'll learn from each other and understand the material better that way. Also try to do work in preparation for Thursday's class before Wednesday since it's sometimes hard to get it all done in one night with other coursework to take care of as well."
Topics to be covered:

*Fundamentals of Quantum Mechanics*

Why do we need quantum mechanics?
The Stern-Gerlach experiment, NMR, and two-state quantum systems
The postulates of quantum mechanics
The classical wave equation and the Schrodinger representation of quantum mechanics

*Basic One-Body Chemical/Molecular Problems*

The quantum particle in a box model
Multidimensional confinement, finite barriers, and tunneling; finite difference theory
The quantum harmonic oscillator and the quantum rigid rotor
Vibrational and rotational spectroscopy, and spectroscopic selection rules
Angular momentum in rotors, NMR, and atoms
The hydrogen atom

*Approximation Methodology and Molecular Structure*

Quantum mechanical approximation methods: variational method and perturbation theory
Multielectron atoms and electronic configurations
The Hartree-Fock mean field approximation for multi-electron systems
Computational quantum chemistry: methods and basis sets
Bonding in diatomic molecules
Bonding in polyatomic molecules: Huckel theory, valence bond theory
(if time) Lasers and electronic spectroscopy
(if time) Electronic structure in solids