Chem 3060

Quantum Chemistry & Spectroscopy
Spring 2013

Instructor: Prof. Ryan P. Steele
Office: INSCC 328
Phone: 801-587-3800
Email: ryan.steele@utah.edu
Office hr: Tues 1:00-2:00pm or by appt

Teaching Assistants:
J.D. Herr (Sec 2)
jdh385@gmail.com
350-21 INSCC, office hrs by appt

Justin Talbot (Sec 3)
justin.talbot@utah.edu
305-8 INSCC, office hrs by appt

Course: MWF 10:45-11:35am
HEB 2006
Section 2: T/Th 7:30-8:20am ST 216
Section 3: T/Th 9:40-10:30am JTB 320
Website on Canvas (Campus CIS, https://gate.acs.utah.edu)

Textbook: *Physical Chemistry: A Molecular Approach* (McQuarrie & Simon) ≈$75-85
Note: This text includes several chapters on thermochemistry, which we will not cover in this course. However, this version is nearly the same price as the version that lacks these chapters. It also contains some additional spectroscopy information, which we *will* utilize.

Also useful…
Introduction to Quantum Mechanics (Griffiths)
Principles of Quantum Mechanics (Shankar)
Physical Chemistry (Atkins)

Objectives: Chemistry is a “bottom-up” discipline, in which we posit that what happens at the molecular level dictates macroscopic properties. Whereas your previous chemistry courses likely have been phenomenological (observing what happens), the main goal of physical chemistry is to *explain* what happens at the molecular level. Given an arbitrary chemical principle or reaction, the goal of this course is to provide you with the tools to explain the phenomenon.

Outcomes include:

- understanding the time, length, and energy scales on which chemical processes occur
- understanding the differences between classical and quantum mechanics
- connecting operators to observables
- distinguishing probabilities, amplitudes, averages, expectation values, and observables
- understanding the origin and implications of quantum coherence
- interpreting spectra
- connecting common approximation methods to standard chemical frameworks (Born-Oppenheimer, molecular orbitals)
- developing molecular-level critical thinking skills

Grades: 25% Homework & quizzes
5% Mini-lesson taught by you (in discussion section)
5% Seminar attendance
15% Mid-term exam #1
15% Mid-term exam #2
15% Mid-term exam #3
20% Final exam

Homework: Homework assignments will be given weekly and are due at the start of class every Wednesday. The homework will be collected before lecture begins; *no late homework will be accepted*. Keys will be posted on the course website, and graded homework will be returned in your discussion section by the following Tuesday.

Exams: The majority of your grade in this course will be determined by examinations. The three mid-terms will be in-class exams, which will vary in format. No make-up exams will be administered. Simply put, do not miss an exam. If you have an unavoidable academic conflict, please provide notice at least two weeks prior to the exam date. These conflicts will be evaluated on a case-by-case basis. The final exam date/time is set by the University, and no exceptions will be made.

Lesson: Once each week, a group of 2-4 students will together present a 15-minute mini-lesson in discussion section. The topic, schedule, and grading will be provided by your TA. The format of the lesson should be similar to what you would teach in a course of your own. It should be live (no videos) but can be a "chalk talk", PowerPoint, or some combination of the two. Demonstrations and/or class participation are allowed and encouraged. The 15-minute time limit, however, will be strictly enforced.

Seminar: A portion of your total grade will be based on attendance at two physical chemistry research seminars in the Chemistry department throughout the semester. These seminars occur weekly on Monday afternoons at 4pm in HEB 2006 (same room as our course). You may choose any two to attend, but I will occasionally direct you toward particularly relevant and accessible topics. A short form will be posted on the course webpage; this form must be filled out during the seminar and handed to your professor or TA *in-person* at the end of the seminar. *Since this seminar occurs beyond our scheduled class time, please let me know *in the first week of class* if you have scheduling conflicts.

Attendance: This class meets five days per week (three lectures, two discussions). Your attendance is required at all class meetings. Detailed attendance records will not be kept; however, occasional quizzes and in-class participation records may be kept and will contribute to your grade. My attendance philosophy: Your job is to be present and participate; my job is to make it worth your while to attend.

Disabilities: "The University of Utah seeks to provide equal access to its programs, services, and activities for people with disabilities. If you will need accommodations in the class, reasonable prior notice needs to be given to the Center for Disability Services, 162 Olpin Union Building, 581-5020 (V/TDD). CDS will work with you and the instructor to make arrangements for accommodations." *Please notify me of any requested accommodations within the first week of class.*

Academic Honesty: Collaborating with fellow members of this course is strongly encouraged and will be an essential tool in your progress. All assignments should, however, be completed by you. Furthermore, any form of cheating on exams will not be tolerated. Period. Please refer to the University regulations for more information. (http://www.regulations.utah.edu/academics/6-400.html)

Cell Phones: As a courtesy to me and to your fellow classmates, please turn off cell phones during class. *No cell phones are allowed during exams*. If your cell phone rings or is seen during an exam, you will have the option to keep your phone or your exam…not both.

Homework "Rules": Each week, two additional points will be given for the homework. One point will be given for legibility; one will be given for following rules 2-4. These points are given at the sole discretion of your TA.

1. Print legibly. We can only grade what we can read. If your handwriting is hopelessly messy, type your homework.
2. Staple your pages together before submitting your homework.
3. Submit the problems in the same order as presented on the assignment. You may, of course, complete them in any order you wish, but please put them in order for your submission.
4. Do not staple over the problem numbers. Be sure to leave room in the corner of your page for your staple.

About the Course:

Physical chemistry is likely the most fundamental course in your curriculum, and for this reason, it is the most exciting. Rather than accepting that chemistry "just happens," physical chemistry provides an explanation and the possibility of prediction. Physical chemistry is also, historically, the most dreaded course in your curriculum, and I am aware of this reputation. This difficulty is not by design. In fact, I hope that all of you succeed and enjoy the wonderful world of quantum mechanics. However, this course marks a distinct shift in your scientific education. First, it is much more mathematical than any chemistry course that you have taken to date. We will use algebra, calculus, vectors, differential equations, and matrix algebra, and all of these techniques will provide rather abstract representations of chemical systems. Furthermore, quantum mechanics makes a sharp departure from classical notions. This lack of intuition means that we *must* rely on the mathematics, which doubles the difficulty. Therefore, this course will focus on both the conceptual and mathematical sides and attempt to help you connect the two.

"Anyone who is not shocked by quantum theory has not understood it."
 - Neils Bohr

"I think that I can safely say that nobody understands quantum mechanics."
 - Richard Feynman
 (We will approach this course somewhat more optimistically.)

My teaching style will require you to participate. This style will be uncomfortable for some of you, and I fully appreciate this fact. However, I would be doing you a disservice by allowing you to merely observe the course. All of your future endeavors will require you to "perform" verbally, and this course is simply part of this training. The classroom environment *will* be friendly and respectful, allowing you to make mistakes without fear of repercussions or embarrassment. Mistakes are an inherent part of learning, and each mistake exposed during class is one that can be corrected before more public situations. Please respect this environment and your colleagues.

About My Expectations:

This class is an upper-division course, and it is probably the most demanding of the chemistry courses that you will encounter. I expect your effort to match these demands. I expect you to be able to recall material from previous courses and use this information to solve physical chemistry problems. I expect you to internalize the material and be able to apply it to problems not covered in homework assignments. Exam questions may be different from the homework, lectures, and your textbook. This design is not intended to trick you or set you up for failure. It is intended to test your ability to *apply* quantum chemistry principles to new situations, which is the ultimate aim of this course. We will practice such exercises throughout the semester. Some tips for success…

- My lectures are for you, not to hear myself talk. Come to class. I will provide information that goes beyond the textbook and will teach you how to think about physical chemistry problems.
- Physical chemistry is a team sport. Do homework in groups, seek help from colleagues, and provide help to them when they ask. Teaching can be as much of a learning experience as asking.
- If you need help, get help. I have office hours, your TA is available, and you have many intelligent classmates. Take advantage of these resources.
- Your textbook is very good but is not the only source. If the explanation in the text does not make sense to you, seek out other texts at the library or find internet sources. They're free!
- Finally, the onus is on *you* to succeed in this course. Your success is dictated by your effort and ambition, not your professor, not your TA, not your textbook. I will provide all of the necessary tools for you to succeed; it is up to you to make use of them.

Important Dates:

16 Jan (Wed) – Drop deadline
6 Feb (Wed) – Exam I
1 Mar (Fri) – Withdraw deadline
8 Mar (Fri) – Exam II
10 Apr (Wed) – Exam III
26 Apr (Fri) – Final Exam

Course Outline (divisions roughly parallel exam topics):

I. Foundations of Quantum Mechanics
   - Classical mechanics
   - Postulates of quantum mechanics
   - Operators
   - Use and meaning of a wavefunction and the Schrödinger equation

II. Reference Systems
   - Particle in a box
   - Harmonic oscillator
   - Rigid rotor
   - Hydrogen atom

III. Spectroscopy
   - Time-dependent quantum mechanics
   - Vibrational, rotational, and electronic spectroscopies
   - Selection rules
   - Born-Oppenheimer and Franck-Condon approximations

VI. Molecules
   - Multi-electron atoms
   - Slater determinants
   - Molecular orbitals
   - Electron correlation
   - Computational methods

Lecture Schedule:

Date	Topic
7 Jan	Introduction, double-slit experiment
9	Review of classical mechanics
11	Failures of classical mechanics, birth of quantum mechanics
14	Basics of wave equations & differential equations
16	Schrödinger's equation
18	Operators, eigenvalue equations, and orthogonality
21	*No Class – Martin Luther King, Jr. Day*
23	Postulates of quantum mechanics, measurements, and a famous feline
25	Commutation and uncertainty
28	Particle in a box I: Solving Schrödinger equation
30	Particle in a box II: Properties and observables
1 Feb	Particle in a box III: Coherence, uncertainty, and interference
4	Particle in a 2D box, Particle in an open box – tunneling
6	*In-Class Midterm Exam [Covers through 1 Feb]*
8	Harmonic Oscillator I: Problem & setup

11	Harmonic Oscillator II: Solutions & properties
13	Harmonic Oscillator III: 2D oscillator, anharmonicity, and heat transfer
15	Rotational motion and Rigid Rotor
18	*No Class – President's Day*
20	Hydrogen atom I: Hamiltonian and atomic units, separation of variables
22	Hydrogen atom II: Angular pieces
25	Hydrogen atom III: Finishing the wavefunction
27	Hydrogen atom IV: Magnetic quantum number, radial distribution functions, and misc.
1 Mar	Hydrogen atom V: Properties and expectation values, Rydberg states
4	Catch-up and review
6	Quantum Computing
8	*In-Class Midterm Exam #2 [Covers through 4 Mar]*
11	*No Class – Spring Break*
13	*No Class – Spring Break*
15	*No Class – Spring Break*
18	Time-dependent quantum mechanics I: Propagator & examples
20	Time-dependent quantum mechanics II: Connection to spectroscopy
22	Rotational spectroscopy and selection rules
25	Vibrational spectroscopy, selection rules, and normal modes
27	Electronic structure I: Hamiltonian and atomic units
29	Electronic structure II: Separability, exchange, and molecular orbitals
1 Apr	Electronic structure III: Hartree-Fock and variational method
3	Electronic structure IV: Molecules, and Born-Oppenheimer
5	Electronic structure V: Odds & ends
8	Electronic structure VI: Electron correlation and basis sets
10	*In-Class Midterm Exam #3 [Covers through 6 Apr]*
12	Electronic Spectroscopy I: Theory
15	Electronic Spectroscopy II: Examples
17	Nuclear magnetic resonance
19	State occupations: Quantum vs classical, superposition vs temperature
22	Case Study: $NO^+(H_2O)_n$
24	Summary & Review
26 (Fri)	*Cumulative, Final exam 10:30am – 12:30pm*