Syllabus for CHM 544: Quantum Chemistry

MW • DHHC 306 • 8:00–9:15 AM • Fall 2017

http://freitag.creighton.edu/CHM544

Instructor: Dr. Mark Freitag
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Office Hours:

Monday:	9:30–11:00 AM, 2:00–4:00 PM
Tuesday:	11:00 AM–4:00 PM
Wednesday:	9:30–11:00 AM, 2:00–4:00 PM
Thursday:	8:00–11:00 AM, 12:00–4:00 PM
Friday:	by appointment

I will be in during my scheduled office hours, but I am more than happy to see you anytime you find me in the office. You're also welcome to schedule an appointment; just send an email.

Block Time Usage. We have 75 minutes every MW for use in this course. On exam days (see the calendar below), you will have the full time to work on the exam. On other days, class will start at 9:30 AM with an ∼10 minute question-and-answer period. When the Q&A is finished, lecture will begin and continue for approximately 50 minutes. If there is any time remaining at the end of lecture, you are welcome to stay in the room until 9:15 AM to ask more questions or discuss the material.

Textbook. Levine, I.N. *Physical Chemistry*, 6th Ed.; McGraw-Hill: New York, 2008. I view this text primarily as a very good resource; I will assume that you are familiar enough with your pchem text that you can remind yourself of topics covered in that course.

I have drawn from the following books to construct this course, but you are under no obligation to purchase them. I believe the library has all of them available.

- Pauling, L; Wilson, E.B. *Introduction to Quantum Mechanics*, Dover Publications: New York, 1935.

- Levine, I.N. *Quantum Chemistry*, 4th Ed.; Prentice Hall: Englewood Cliffs, NJ, 1991.

- Fitts, D.D. *Principles of Quantum Mechanics*, Cambridge University Press: Cambridge, 1999.

- Atkins, P.W.; Friedman, R.S. *Molecular Quantum Mechanics*, 3rd Ed.; Oxford University Press: New York, 1999.

- Szabo, A.; Ostlund, N.S. *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, McGraw-Hill: New York, 1989.

- Silbey, R.J.; Alberty, R.A. *Physical Chemistry*, 3rd Ed.; John Wiley & Sons: New York, 2000.

- McQuarrie, D.A.; Simon, J.D. *Physical Chemistry: A Molecular Approach*, University Science Books: Sausalito, CA, 1997.

The following are also very good, but I have not drawn on them directly for this course:

- Anderson, *Introduction to Quantum Chemistry*, W.A. Benjamin: New York, 1969.

- Eyring, Walter and Kimball, *Quantum Chemistry*, John Wiley & Sons: New York, 1944.

- McQuarrie, *Quantum Chemistry*, University Science Books: Mill Valley, CA, 1983.

- Pople and Beveridge, *Approximate Molecular Orbital Theory*, McGraw-Hill: New York, 1970.

Introduction/Attendance. Attendance in lecture is highly recommended, but not required. Keep in mind that you are still responsible for all information given in lecture even if you are not present.

Course Objectives. Students will. . .

- know the postulates of quantum mechanics.

- be able to solve Schrödinger's equation for the hydrogen atom.

- be able to describe quantized angular momentum using ladder operators.

- understand how electron spin is incorporated into the spatial wave function.

- be able to solve Schrödinger's equation for H_2^+ using LCAO-MO theory.

- understand the variational theorem.

- be able to derive the Hartree-Fock Self-Consistent Field equations.

Exams: Logistical Details. The tentative exam dates are given in the *Course Timeline* below. Plan on taking the exam on the given date. I will make other arrangements if you have an officially excused absence for University-sponsored affairs cleared with the Dean's office. If for any reason you cannot make it at the scheduled time, you must contact me at least one week before the exam. This does not necessarily mean that your absence will be excused, but if you fail to notify me in advance, you will not be able to reschedule the exam under any circumstances. Of course, emergencies and unforeseen circumstances will be considered on an individual basis. ("*I couldn't find a babysitter*," and "*I don't feel well*" are not emergencies—car accidents, snowstorms and other Acts of God are.)

The final exam will only cover the material from the previous exam; i.e., it will *not* be comprehensive.

Extra Help. If for some reason you can't stop by my office, send an email. I should be able to reply fairly promptly (except at night and on weekends; then you might have to wait a day or so). If you have other suggestions for added help, please let me know and I shall try to incorporate them.

Grading. All the points in this course will come from the following sources:

Item	Points
Four hour exams, 100 pts each	400
Problem sets	100
Total	500

I do not have strict, predetermined cutoffs for letter grades; instead, I look for natural breaks in the distribution of course scores. However, I will use the following as a starting point:

A	B+	B	C+	C	D
90%	87%	80%	77%	70%	60%

These cutoffs are never increased. Course grades are rounded to the nearest whole number. You may ask about your grade over email, but because of privacy issues I can only reply if you send your question from your Creighton University account.

Academic Honesty. Creighton University has an established policy on academic honesty. You can read about it at your leisure in the Catalog.[*] If you're in this class, you've been around the block a time or two and you know what it is. Don't do anything foolish. If you do, I'll probably find out and then have to give you a zero for the activity.

Parting Thoughts. Don't procrastinate, and don't be lazy. If you feel yourself falling behind, please come and see me even if you can't identify a specific problem. I should be able to tell where you're at progress-wise. If I think you're doing fine, I'll say so. If not, we'll try to figure out how to get you back up to speed. Take advantage of the resources that are available (myself, discussion groups, posted notes, etc.). If you require some other form of assistance, please don't hesitate to ask. I am here to help in any way I can.

A final suggestion: unplug. Technology can be a good thing, but it can also be a mindless distraction and—despite its potential for the opposite—a lonely, detached waste of time. When it comes to technology, exercise prudence: just because you *can* do something electronically doesn't mean it's the best way to do it. Also exercise temperance: if you can't go two minutes without fiddling with your smartphone, leave teddy at home. While you're on campus, allow yourself the time and silence to simply *think*.

Course Timeline. The following is a tentative timeline and topics for the course. Some of the dates and coverage may change.

MONDAY	WEDNESDAY
21 August	23 1 The Postulates of Quantum Mechanics

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[*] http://catalog.creighton.edu/undergraduate/academic-policies-procedures/academic-honesty/

MONDAY		WEDNESDAY	
28	2	30	3
The Postulates of Quantum Mechanics, con't.		The Postulates of Quantum Mechanics, con't.	
4 September	3	6	4
Labor Day – No class		The Heisenberg Uncertainty Principle and Simultaneous Eigenfunctions	
11	5	13	6
The Hydrogen Atom		**Exam I: 23 Aug–6 Sep**	
18	7	20	8
The Hydrogen Atom, con't.		The Hydrogen Atom, con't.	
25	9	27	10
The Hydrogen Atom, con't.		The Hydrogen Atom, con't.	
2 October	11	4	12
The Rigid Rotor and Angular Momentum		**Exam II: 11–27 Sep**	
9	13	11	14
The Rigid Rotor and Angular Momentum, con't.		The Rigid Rotor and Angular Momentum, con't.	
16		18	
Fall Break – No class		**Fall Break** – No class	
23	15	25	16
The Rigid Rotor and Angular Momentum, con't.		Electron Spin and the Helium Atom	
30	17	**1 November**	18
Electron Spin and the Helium Atom, con't.		The Variational Method	
6	19	8	20
Exam III: 2–30 Oct		LCAO-MO Theory	
13	21	15	22
The Hydrogen Molecule-Ion		The Hydrogen Molecule-Ion, con't.	
20	23	22	
Hartree Products and Exchange Repulsion		**Thanksgiving Break** – No class	
27	24	29	25
The Hartree-Fock Self-Consistent Field Method		The Hartree-Fock Self-Consistent Field Method, con't.	
4 December	26	6	27
The Hartree-Fock Self-Consistent Field Method, con't.		The Hartree-Fock Self-Consistent Field Method, con't.	

Exam IV: 1 Nov–6 Dec
Monday, 11 Dec 2017, 9:30–10:45 AM