

CHM4412 — Physical Chemistry – Quantum Chemistry

Instructor	Dr. Alexander Angerhofer (Dr. A)
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E-mail	alex@chem.ufl.edu
Class Times	T,R-3+4 periods (9:35-11:30am) in Fine Arts Bldg. C, room 127
Office Hours	T-7 (1:55 – 2:45pm), W-8 (3:00 – 3:50pm), R-5 (11:45am – 12:35pm) in CLB318A

TA	Anthony Pastore	Shalini Jayaraman Rukmani
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Office Hours	M-7, W-7, F-2 periods (CLB 318), and by appointment	M-9, W-9, F-7 periods (FLI 258), and by appointment

Holidays	01/18 (MLK Day), 02/27-03/04 (Spring Break), 04/21-22 (Dead Week, no classes).	
Class Text	Kuhn, Försterling, Waldeck, Principles of Physical Chemistry, 2 nd Edition, John Wiley & Sons, Hoboken NJ, 2009, ISBN: 978-0-470-08964-4.	
Homework	Homework will be assigned weekly except during weeks of mid-term exams, and will involve solving problems assigned by the instructor. Homework will be graded.	
Points Earnable	3 progress exams @ 200 pts. each for 600 pts. total. 1 optional cumulative final exam @ 400 pts. For 400 pts total. 10 homeworks @ 30 pts. each for 300 pts. total. 3 online quizzes @ 50 pts. each for 150 pts. total. 1 participation grade @ 150 pts. for 150 pts. total. Total earnable points are 1,600 pts. with and 1,200 pts. without final exam.	
Grading Scheme	<p>With final exam:</p> <p>A: ≥ 1360 pts. (85.0%) $1360 \text{ pts} > A- \geq 1320$ pts. (82.5%) $1320 \text{ pts} > B+ \geq 1280$ pts. (80.0%) $1280 \text{ pts} > B \geq 1200$ pts. (75.0%) $1200 \text{ pts} > B- \geq 1160$ pts. (72.5%) $1160 \text{ pts} > C+ \geq 1120$ pts. (70.0%) $1120 \text{ pts} > C \geq 1040$ pts. (65.0%) $1040 \text{ pts} > C-^{\ddagger} \geq 1000$ pts. (62.5%) $1000 \text{ pts} > D+ \geq 960$ pts. (60.0%) $960 \text{ pts} > D \geq 880$ pts. (55.0%) $880 \text{ pts} > E$.</p>	<p>Without final exam</p> <p>A: ≥ 1020 pts. $1020 \text{ pts} > A- \geq 990$ pts. $990 \text{ pts} > B+ \geq 960$ pts. $960 \text{ pts} > B \geq 900$ pts. $900 \text{ pts} > B- \geq 870$ pts. $870 \text{ pts} > C+ \geq 840$ pts. $840 \text{ pts} > C \geq 780$ pts. $780 \text{ pts} > C- \geq 750$ pts. $750 \text{ pts} > D+ \geq 720$ pts. $720 \text{ pts} > D \geq 660$ pts. $660 \text{ pts} > E$.</p>

[‡] please note that a 'C-' is not considered a passing grade for majors requiring this course.

Course Schedule (tentative):

Date	Day	Chapter	Topic	Reading
01/05/16	T	1	Mathematical Tools of Physical Chemistry	
01/07/16	R	1	Wave-Particle Duality, Electrons	pp. 3-20
01/12/16	T	2	Atomic Line Spectra	pp. 21-30
01/14/16	R	2	Aspects of Structure and Bonding	pp. 30-41
01/19/16	T	3	Schrödinger Equation	pp. 42-57
01/21/16	R	3	Properties of Wavefunctions	pp. 57-75
01/26/16	T	4	Hydrogen Atom Ground State	pp. 76-82
01/28/16	R	4	Hydrogen Atom Excited States	pp. 82-92
02/02/16	T	5	The Variational Principle	pp. 93-104
02/03/16	W	1 – 4	1 st Mid-Term Exam (periods E2 – E3, place tba)	
02/04/16	R	5	Electron Spin	pp. 104-115
02/09/16	T	5	The Aufbau Principle and the Periodic Table	pp. 115-127
02/11/16	R	6	The H ₂ ⁺ Molecule	pp. 128-139
02/16/16	T	6	The H ₂ Molecule	pp. 139-149
02/18/16	R	7	Electron Pair Bonds	pp. 150-161
02/23/16	T	7	Molecular Orbitals	pp. 161-177
02/25/16	R	7	Molecular Properties	pp. 177-188
03/08/16	T	8	Molecules with π -Electrons	pp. 189-209
03/10/16	R	8	HMO Theory	pp. 209-219
03/15/16	T	9	Excitation of π -Electron Systems	pp. 220-235
03/16/16	W	5 – 8	2 nd Mid-Term Exam (periods E2 – E3, place tba)	
03/17/16	R	9	Structural Effects on Absorption	pp. 235-249
03/22/16	T	9	Optical Activity	pp. 249-260
03/24/16	R	10	Fluorescence and Phosphorescence	pp. 261-275
03/29/16	T	10	Stimulated Emission and Laser Principle	pp. 275-279
03/31/16	R	11	Rotational Spectroscopy	pp. 280-293
04/05/16	T	11	Vibrational Spectroscopy	pp. 293-315
04/07/16	R	11	Raman Spectroscopy	pp. 315-324
04/12/16	T	11	Electronic Spectroscopy	pp. 324-336
04/13/16	R	12	Nuclear Magnetic Resonance	pp. 337-350
04/19/16	T	12	Electron Spin Resonance	
04/20/16	W	9 – 12	3 rd Mid-Term Exam (periods E2 – E3, place tba)	
04/27/16	M	1—12	Cumulative Final Exam 5:30—7:30pm	

Further Important Information:

1. **Overview and Goals:** CHM 4412 introduces quantum theory, atomic and molecular structure, chemical bonding and spectroscopy.
2. **Prerequisites:** One year of General Chemistry (CHM2045/46, CHM2045/51, CHM2047, or equivalent) and one year of college physics or equivalent (ideally PHY2048/49), background in analytical (CHM3120) and organic chemistry (CHM2210/11, CHM2212/13, or CHM3217/18) is recommended. CHM4411 is not a prerequisite.
3. **Corequisites:** MAC2313 (implies MAC2311/12 as prerequisites).
4. **Exam Dates:** All during-term exams are evening exams taking place during periods E2+E3 (8:30pm – 10:10pm). Dates for the three exams are: February 03; March 16; April 20. The final exam date is May 1st and will take place in FAC 127 from 5:30pm – 7:30pm (exam group 27E).
5. **Exam Policies:** Three during-term exams will be given (see schedule above). These exams will be evening exams. Exam duration will be approximately 2 hours. Making up a missed exam is a serious and exceptionally burdensome problem. Consequently, a makeup exam will require that you have a legitimate excuse, and that you have brought this to the attention of the instructor before the missed exam. Legitimate excuses include sickness or a conflict with another exam for a higher numbered class. If you are not sure whether your excuse is valid, talk to the instructor before missing an exam. If you have an emergency that prevents you from letting the instructor know ahead of time, an excused absence and rescheduled make-up exam will be granted after official documentation about your emergency (doctor's notes, *etc.*) deemed appropriate by your instructor has been presented.

The final exam is optional. If a student is happy with his/her grade at the end of the semester (see grading scale without final exam above) he/she may skip the final exam. Since the final exam is cumulative, the instructor reserves the right to consider assigning a letter grade above that which the student would receive based strictly on total points earned (as listed above). This will only take effect if the final exam is taken and the performance on the final exam is significantly above the student's overall performance for the semester, and if the student shows clear improvement in his/her exam grades over the course of the semester. This qualification cannot lower your grade and will depend on the instructor's evaluation of the student's performance on the final exam.

A student contending that an exam or quiz has been mis-graded or mis-scored must report this to the TA responsible for grading within one week of receiving the original grade or score. Failure to follow this policy results in no reconsideration of the contended grade or score. For all questions on grades or grading, please consult with the TA first in person. If this does not resolve the issue you may talk to the instructor about it. Except for problems with on-line quizzes (see below), emailed questions on grades or grading will not be answered.

6. **Calculators:** You must have your own scientific calculator. Calculators may be used on quizzes and exams but may not be shared. You may not use graphing calculators or any calculators that are capable of information storage or communication on any exam. Simple inexpensive scientific calculators such as the TI-30 series or the Casio fx-260 are acceptable and sufficient for any problem encountered on exams.
7. **On-line Quizzes:** There will be three on-line quizzes on elearning (1 quiz = 50 points max.). The on-line quizzes will be administered through the canvas elearning interface to the class. Quiz durations will be between 30 and 60 minutes depending on the level of difficulty and the number of questions. For your convenience the web format will allow for an extended period of time (typically a 4-day period) during which you can take the quiz. Once a quiz has been started the clock starts running and you have to finish it in the allotted time. On-line quizzes will typically open up the Friday before a mid-term exam and close the following Tuesday night.
8. **Elearning:** This course uses the canvas e-learning site. Please log on at <http://elearning.ufl.edu> to get access to your course page.

9. **Homework:** Homework (HW) will be assigned weekly and problem sets posted on canvas. HW problems come from many different sources, including the instructor's own personal list of problems. Assignments will typically be available on canvas by Wednesday night and are due the Thursday of the following week at the beginning of lecture (9:35am). Policies for late submission: Each work day that HW is late, 20% of the achievable points are subtracted. It is considered a day late if it is turned in after 9:35am the day it is due. Do your HW! By doing HW problems you will collect essential points toward your grade and will be better prepared to deal with problems on exams.
10. **Participation Grade:** The participation points (up to 150) will be earned through active participation in class. This is primarily done by using the learning catalytics app on your digital device (smartphone, tablet, notebook PC, *etc.*) to respond to questions asked by the instructor throughout the lectures (see further explanation below under #12).
11. **Learning Catalytics (LC):** In this course, we will use LC for your digital device for you to respond to the instructor's questions and earn valuable points toward your grade. You will need to purchase access and create a student account on <https://learningcatalytics.com/>. Follow instructions on the web site, or in the registration document on your Canvas account (click on Files → LC → Get_Started_Flyer_Learning_Catalytics.pdf) to activate your account and link it to our course, CHM4412. The cost is \$12 for the semester. You are required to bring at least one wifi-enabled digital device to class to use for this activity. If you don't have access to a digital device, please contact the instructor.
12. **Study Habits:** This course requires on average 8 – 10 hours/week of work outside of class. Regular lecture attendance is essential. The class will not be taught “by the book.” It is expected that you read the assigned pages from the textbook in advance to coming to class. The instructor will build on this material and you are expected to be able to follow in-class discussion. The course demands a regular sustained effort throughout the term. Most importantly, do not allow yourself to fall behind! The material builds up and you need to stay ahead of the game. If you find that you are not grasping essential material by reading the textbook and following in-class discussion, seek help! Visit your instructor's and/or TA's office hours (see above), talk to other students in your class, compare notes, form a study group, *etc.*
13. **Class Attendance:** Lecture attendance is essential for your success in this class. However, we will not take roll-calls. Repeated absence in class will make it very difficult to earn full participation points (see above).
14. **Students with Disabilities:** Students requiring special accommodations should register with the Dean of Students Office and present documentation from that office to the instructor.
15. **Counseling Services:** The University of Florida provides counseling services for students, staff, and faculty. See <http://www.counsel.ufl.edu/> or call (352) 392-1575 during regular service hours (8am – 5pm). For other hours or on weekends call the Alachua County Crisis Center (264-6789). Students may also call the clinician on-call at Student Mental Health for phone callback and consultation at (352) 392-1171.
16. **Cell Phones:** Please put all cell phones and other digital devices on “silent mode” during all class periods. Thank you.
17. **Honors Code:** This class will operate under the policies of the student honor code which can be found at: <http://www.registrar.ufl.edu/catalog/policies/students.html> The students, instructor, and TA's are honor-bound to comply with the Honors Pledge: **We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.**

If you have further questions, please contact me. Have a great semester!

Sincerely, Alexander Angerhofer