

Chem 4502 **Introduction to Quantum Mechanics and Spectroscopy** 3 Credits
Fall Semester 2018

Prerequisites: Two prior semesters of chemistry, two prior semesters of physics, two prior semesters of calculus.

Time: MWF 10:10 – 11:00
Location: Smith Hall 231, TCEASTBANK

Instructor: Laura Gagliardi (229 Smith Hall, gagliard@umn.edu)

TA:
Christian Hettich (hetti029@umn.edu)
Sam Stoneburner (101 Smith Hall, sstonebu@umn.edu)

Office Hours:

Laura Gagliardi:	M	2:00-4:00 pm	101 J Smith Hall
Christian Hettich:	Th	3.00-5.00 pm	Kolthoff 285

Textbook: There is no required textbook. Daily class lectures will be distributed on the class website as pdf files. An *optional* book available in the bookstore is McQuarrie and Simon *Physical Chemistry A Molecular Approach*, University Science Books, 1997.

Class Website: <http://www.chem.umn.edu/groups/gagliardi/teaching.html> site will include at a minimum all class materials. Note that you are welcome to use the upper division microcomputer lab 101D Smith Hall if you want to print class materials free of charge.

Coursework: The class is lecture-like in format, with the anticipated topics to be covered outlined below. Students are expected to keep up with posted class readings (they'll be made available at least a few days in advance) and to work on assigned homework problems (see below). My intent is to spend the first 5 to 10 minutes of each lecture going over a previously assigned problem, and the remainder on lecture/demonstration of new material. Classroom attendance is not required, but you are likely to have a *much* more difficult time if you fail to attend classes.

Homework: At the end of each day's lecture notes will be 2 homework problems. I will discuss the solution to the *first* of the problems at the start of the following lecture. Students should do the problem but will not be expected to turn in their work or solutions. The *second* homework problem, on the other hand, should be prepared to be turned in for grading. Once a week, (**usually each Friday, but check the schedule below because sometime it will be a different day of the week**) at the start of class, the solutions to all *second* homework problems will be collected. One of these, selected at random, will be graded carefully, while the other(s) will be more cursorily checked. Answer keys will be provided online after the graded homework is collected. ***As a result, no homework will be accepted after the class period in which it is due. You can consult any material available, when solving the homework problems. However, you are supposed to elaborate your problems on your own. If some homework appears to be copied verbatim from any existing source, it will receive zero points.***

Exams: Exams will be cumulative on all class materials up to that point, with heavy emphasis on new material covered since any prior exam. The final exam will cover the entire semester, with some additional emphasis on topics covered in the last two weeks of

class (for which no in-term exam is scheduled). The format of the exams will combine multiple choice with one or two short problems chosen to have close correspondence to assigned homework. Arriving at the answer to either type of problem may well involve some mathematical calculations; space and relevant formulae required to perform such calculations will be provided. Exams will likely be given in two rooms. Room assignments will be announced in class. The exams will emphasize *conceptual* details over mathematical manipulations, but testing on a certain amount of the latter cannot be avoided.

Grading: There will be 4 exams during the semester and a final exam on **Thursday, Dec. 20 from 1:30 p.m.-3:30 p.m.** Your lowest score will be dropped and the remaining 3 in-term exams will constitute 60% of your final grade. Graded homework will count for 10%, and the final exam will constitute the remaining 30% of your final grade. If you miss an exam, for whatever reason, the missed exam will be the dropped exam. If, through outrageous fortune, you are forced to miss *two* exams, we can discuss remedies at the appropriate time. ***Under no conditions will it be possible to reschedule the final exam, nor can that exam somehow be dropped.*** The class will be graded on an **absolute scale:** The total number of possible points in the course is 500, and you must earn at least 400 points for an A-, 350 points for a B-, 275 points for a C-, and 250 points for a D. Thus, earning approximately 80% of possible points enters the A range, 70% the B range, 55% the C range, 50% the D range, and earning less than 50% of possible points will result in a failing grade. As warranted, “+” and “-” grades will be awarded within each range based on the overall performance of the class. Notice that there is no A+ grade (see **Grading and Transcripts** below). The separation between A- and A will be decided based on the overall performance of the class.

Calculators: No calculators, nor any other electronic devices, will be allowed during exams. You will be provided with all formulae required to solve problems (e.g., solutions to non-trivial integrals) and answers will be expressed in terms of constants that need not be reduced to decimal values.

Preparing for Exams: The most effective method to prepare for an exam is to study the lecture notes, the assigned problems, and the textbook. I am happy to discuss any of these items during office hours, as is the TA, if you need feedback.

The following material has been adapted from:

<https://policy.umn.edu/education/syllabusrequirements>

Student Conduct Code: The University seeks an environment that promotes academic achievement and integrity, that is protective of free inquiry, and that serves the educational mission of the University. Similarly, the University seeks a community that is free from violence, threats, and intimidation; that is respectful of the rights, opportunities, and welfare of students, faculty, staff, and guests of the University; and that does not threaten the physical or mental health or safety of members of the University community.

As a student at the University you are expected adhere to Board of Regents Policy: *Student Conduct Code*. To review the Student Conduct Code, please see: http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student_Conduct_Code.pdf.

Note that the conduct code specifically addresses disruptive classroom conduct, which means "engaging in behavior that substantially or repeatedly interrupts either the instructor's ability to teach or student learning. The classroom extends to any setting

where a student is engaged in work toward academic credit or satisfaction of program-based requirements or related activities."

Use of Personal Electronic Devices in the Classroom

Using personal electronic devices in the classroom setting can hinder instruction and learning, not only for the student using the device but also for other students in the class. To this end, the University establishes the right of each faculty member to determine if and how personal electronic devices are allowed to be used in the classroom. For complete information, please reference: <http://policy.umn.edu/education/studentresp>.

Scholastic Dishonesty

You are expected to do your own academic work and cite sources as necessary. Failing to do so is scholastic dishonesty. Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis. (Student Conduct Code: http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student_Conduct_Code.pdf)

If it is determined that a student has cheated, the student may be given an "F" or an "N" for the course, and may face additional sanctions from the University. For additional information, please see: <http://policy.umn.edu/education/instructorresp>.

The Office for Community Standards has compiled a useful list of Frequently Asked Questions pertaining to scholastic dishonesty: <https://communitystandards.umn.edu/avoid-violations/avoiding-scholastic-...>. If you have additional questions, please clarify with your instructor for the course.

Makeup Work for Legitimate Absences

Students will not be penalized for absence during the semester due to unavoidable or legitimate circumstances. Such circumstances include verified illness, participation in intercollegiate athletic events, subpoenas, jury duty, military service, bereavement, and religious observances. Such circumstances do not include voting in local, state, or national elections.

For complete information, please see: <http://policy.umn.edu/education/makeupwork>.

Appropriate Student Use of Class Notes and Course Materials

Taking notes is a means of recording information but more importantly of personally absorbing and integrating the educational experience. However, broadly disseminating class notes beyond the classroom community or accepting compensation for taking and distributing classroom notes undermines instructor interests in their intellectual work product while not substantially furthering instructor and student interests in effective learning. Such actions violate shared norms and standards of the academic community. For additional information, please see: <http://policy.umn.edu/education/studentresp>.

Grading and Transcripts

The University utilizes plus and minus grading on a 4.000 cumulative grade point scale in accordance with the following:

A	4.000
A-	3.667
B+	3.333

B	3.000
B-	2.667
C+	2.333
C	2.000
C-	1.667
D+	1.333
D	1.000
S	.

For additional information, please refer to:
<http://policy.umn.edu/education/gradingtranscripts>.

Sexual Harassment

"Sexual harassment" means unwelcome sexual advances, requests for sexual favors, and/or other verbal or physical conduct of a sexual nature. Such conduct has the purpose or effect of unreasonably interfering with an individual's work or academic performance or creating an intimidating, hostile, or offensive working or academic environment in any University activity or program. Such behavior is not acceptable in the University setting. For additional information, please consult Board of Regents Policy: https://regents.umn.edu/sites/regents.umn.edu/files/policies/Sexual_Harassment_Sexual_Assault_Stalking_Relationship_Violence.pdf

Equity, Diversity, Equal Opportunity, and Affirmative Action

The University provides equal access to and opportunity in its programs and facilities, without regard to race, color, creed, religion, national origin, gender, age, marital status, disability, public assistance status, veteran status, sexual orientation, gender identity, or gender expression. For more information, please consult Board of Regents Policy: http://regents.umn.edu/sites/regents.umn.edu/files/policies/Equity_Diversity_EO_AA.pdf.

Disability Accommodations

The University of Minnesota views disability as an important aspect of diversity, and is committed to providing equitable access to learning opportunities for all students. The Disability Resource Center (DRC) is the campus office that collaborates with students who have disabilities to provide and/or arrange reasonable accommodations.

- If you have, or think you have, a disability in any area such as, mental health, attention, learning, chronic health, sensory, or physical, please contact the DRC office on your campus (UM Twin Cities - [612.626.1333](tel:612.626.1333)) to arrange a confidential discussion regarding equitable access and reasonable accommodations.
- Students with short-term disabilities, such as a broken arm, **can** often work with instructors to **minimize** classroom barriers. In situations where additional assistance is needed, students should contact the DRC as noted above.
- If you are registered with the DRC and have a disability accommodation letter dated for this semester or this year, please contact your instructor early in the semester to review how the accommodations will be applied in the course.
- If you are registered with the DRC and have questions or concerns about your accommodations please contact your (access consultant/disability specialist).

Additional information is available on the DRC website: sdzavada@r.umn.edu, UM Twin Cities - drc@umn.edu with questions.

Mental Health and Stress Management

As a student you may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance and may reduce your ability to participate in daily activities. University of Minnesota services are available to assist you. You can learn more about the broad range of confidential mental health services available on campus via the Student Mental Health Website: <http://www.mentalhealth.umn.edu>.

Academic Freedom and Responsibility: *for courses that do not involve students in research*

Academic freedom is a cornerstone of the University. Within the scope and content of the course as defined by the instructor, it includes the freedom to discuss relevant matters in the classroom. Along with this freedom comes responsibility. Students are encouraged to develop the capacity for critical judgment and to engage in a sustained and independent search for truth. Students are free to take reasoned exception to the views offered in any course of study and to reserve judgment about matters of opinion, but they are responsible for learning the content of any course of study for which they are enrolled.* Reports of concerns about academic freedom are taken seriously, and there are individuals and offices available for help. Contact the instructor, the Department Chair, your adviser, the associate dean of the college, or the Vice Provost for Faculty and Academic Affairs in the Office of the Provost.

Laura Gagliardi

COURSE OUTLINE

Date	Topic/Reading
W 09/05	L1 Discussion of Syllabus. Origins of quantum hypothesis, blackbody radiation, photoelectric effect, hydrogen atom line spectra. Philosophical environment of science at that time.
F 09/07	L2 One-electron atomic model. Wave-particle duality. The de Broglie wavelength.
M 09/10	L3 The Schrödinger wave equation. Probability and quantum mechanics. Collapse of the wave function upon sampling.
W 09/12	L3 Continues (Active Learning)
F 09/14	L4 Matrix and vector interpretation of wave functions and operators. Key linear algebraic details associated with quantum mechanics. Complex numbers. Dirac notation. The turnover rule. Homework 1 due.
M 09/17	L5 Stationary states. Operators and their expectation values. The Uncertainty principle.
W 09/19	L6. Free particles and the particle in a box.
F 09/21	Catch-up and review. Homework 2 due.
M 09/24	Exam I (You will be tested up to lecture 6) Locations: 231 Smith and Armory 202
W 09/26	L7 Spectroscopy of the particle in a box. Parity. Selection rules. QM tunneling out of a box with one wall of finite height and width.
F 09/28	L8 The QM harmonic oscillator. Homework 3 due.
M 10/01	L9 The QM harmonic oscillator continued. Zero-point energy. Infrared spectroscopy. (Active Learning)
W 10/03	L10 Angular momentum, classical and QM. Polar coordinates. Raising and lowering operators. Eigenvalues of L_z and L^2 .
F 10/05	L11 Angular momentum eigenfunctions. The spherical harmonics. Homework 4 due.
M 10/08	Catch-up and review.
W 10/10	L12 Spectroscopy of the rigid rotator. Diffuse interstellar bands.
F 10/12	Catch-up and review. Homework 5 due.
M 10/15	Exam II (You will be tested up to lecture 12) Locations: 231 Smith and Armory 202

- W 10/17 L 13 Research presentation: What's Quantum Chemistry Good For?
- F 10/19 L14 The QM hydrogen atom.
- M 10/22 L15 Hydrogenic orbitals.
- W 10/24 L16 Spectroscopy of the hydrogen atom. Electron spin. Spin-orbit coupling. The Zeeman effect. Electron-spin resonance spectroscopy.
- F 10/26 **Catch-up and review. Homework 6 due.**
- M 10/29 L17 The variational principle. The Born-Oppenheimer approximation. Basis functions.
- W 10/31 L18 Examples of variational calculations. The helium atom. (Active Learning)
- F 11/02 L19 More variational calculations. The hydrogen atom. Gaussian basis sets. **Homework 7 due.**
- M 11/05 Catch up and review.
- W 11/07 L20 Antisymmetry. Fermions and bosons. Spin.
- F 11/09 **Exam III (You will be tested up to Lecture 19)**
Locations: 231 Smith and Armory 202
- M 11/12 L20 Antisymmetry. Fermions and bosons. Spin Continued
- W 11/14 L21 Two-electron wave functions. Hartree products. The Slater determinant. Many-electron wave functions. Spin orbitals.
- F 11/16 L22 Spin algebra. Singlet and triplet states. **Homework 8 due.**
- M 11/19 L22 Continued. The Helium atom revisited. (Active Learning)
- W 11/21 L23 Review and Catch Up.
- F 11/23 **THANKSGIVING WEEKEND NO CLASS**
- M 11/26 L24 Recap of variational principle and LCAO approach. Solution of the secular equation. Effective Hamiltonians. Hückel theory. **Homework 9 due.**
- W 11/28 L25 Many-electron Wave Functions. Hartree Products. (Active Learning)
- F 11/30 L26 Spin review. The Hartree-Fock method.
- M 12/03 L27 The Hartree-Fock Self-Consistent Field Procedure.
- W 12/05 L28 The Water molecule at the HF level.
- F 12/07 What is the highest bond order in the periodic table? **VISIT TO MSI computers Homework 10 due.**
- M 12/10 **Catch-up and review.**
- W 12/12 **Exam IV (You will be tested up to L 28)**
Locations: 231 Smith and Armory 202
- Th 12/20 FINAL Thursday, Dec. 20 from 1:30 p.m.-3:30 p.m** Fraser 101 (Cap. 192).