

CHEM 4511W - Advanced Physical Chemistry Laboratory

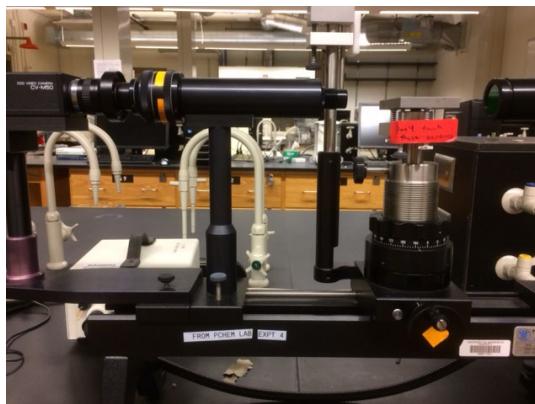
Fall, 2023 - 3 Credits

Instructor:

Professor Ken Leopold
217 Smith Hall
612 625-6072
kleopold@umn.edu

TAs:

Connor Reilly (reill279@umn.edu)
Luis Padilla (padil123@umn.edu)



Location and Times:

Lecture: M 1:25 PM – 2:15 PM, 11 Appleby Hall

Lab: T 1:25 – 5:15 PM, Kolthoff Hall 465 (section 2)
W 1:25 – 5:15 PM, Kolthoff Hall 465 (section 3)

Prerequisites:

CHEM 4502, Chemistry Major

Special Considerations Due to COVID-19:

Up-to-date policy information is available on the [Safe Campus Covid Page](#). The University expects all community members to respect those who choose to wear a mask, as well as those who choose not to wear one. I may often wear a mask in class, and I fully support your individual choices around masking.

Note that if you are showing symptoms that may be due to Covid, or if you have been exposed and need to quarantine, please do not come to lab. This will be treated as not only a responsible action, but as a legitimate excused absence for which there will be no penalty. Our lab schedule is flexible and there will be ample time for makeup labs!

General Course Information:

Welcome to CHEM 4511W, the Advanced Physical Chemistry Laboratory! Chemists, like all scientists, are trying to make sense of the world around them. One important approach to this involves the application of basic physical principles to chemical problems. In physical chemistry, we do just that. But remember that all theories, no matter how simple or complex, are ultimately rooted in experiment. In the physical chemistry laboratory, you will perform a variety of experiments that illustrate the process. Moreover, our measurements allow us to make remarkable statements about the invisible, microscopic world.

This course will expose you to a variety of experiments in physical chemistry and provide you with a hands-on reinforcement of fundamental topics developed throughout the Physical Chemistry lecture courses (e.g., quantum mechanics, spectroscopy, thermodynamics, equilibrium, and reaction kinetics). To accomplish this requires developing a particular set of skills that include collecting, assessing, and analyzing quantitative data. Development of these skills will be a strong focus this semester.

Writing Intensive Course:

CHEM 4511W is a Writing Intensive course. Having strong writing skills is a huge part of being a successful scientist. Whether you go into industry, academics, government, teaching, public policy, medicine, or law, you will need to be an articulate messenger in order to communicate your thoughts, intentions, and accomplishments. Different fields have different styles of written communication, and science is no exception. We will focus hard on high quality scientific writing. This means that, in addition to addressing chemical content, you will be writing (and will be graded on) scientific journal-style short papers describing your experiments, results, and interpretations. We will particularly emphasize *writing style, error analysis, proper presentation of data (graphical and tabular), as well as knowing what and how much information should be included in a scientific report in order to enable others to replicate your results.*

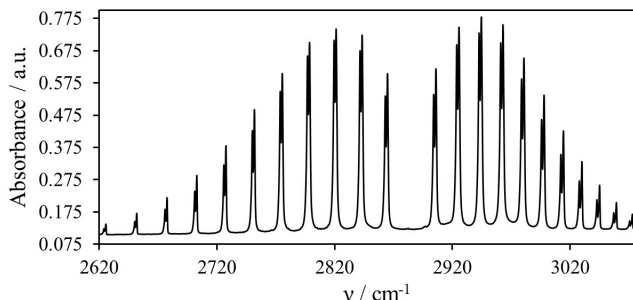
Note that writing, like most skills, is best learned through practice and iteration. To help with this, you will be submitting first drafts of your writing for some of the lab reports. These will be “graded” by the TAs to provide feedback that you can use to produce your best work in the final version. Scientific writing will be discussed in the lecture early in the semester, and separate documents will be provided with advice and instructions. Please don’t hesitate to ask the TAs or the instructor questions regarding writing style, content, etc.

Required Course Materials and Website:

All required course materials are available on the class Canvas site
<https://canvas.umn.edu/courses/390632>

Additional Useful Resources:

Because CHEM 4502 is a prerequisite for the class, you likely have access to a physical chemistry textbook. *Physical Chemistry*, by McQuarrie and Simon, is sufficient. For clarification, alternate perspectives, or different writing styles, there are many other excellent texts that you can find in the library. The books *Quantum Chemistry* by McQuarrie and *Molecular Quantum Mechanics* by Atkins and Friedman are recommended. There are many other excellent books in the library that you can choose from. We will, on occasion, also be using journal articles as resources.



There will be times in this course when you will need to look up data from the literature. There are many available resources that should help you do so. Meghan Lafferty, the librarian at the U of M with special expertise in chemistry, has put together a great website specifically designed for CHEM 4511W:

<https://libguides.umn.edu/CHEM/4511W>

Meghan is also happy to answer questions and provide assistance. Her email address is mlaffert@umn.edu.

SciFinder is also a useful resource, but we have now upgraded to Scifinder-n. If you have *already* established a SciFinder username and password, click on the link below to access SciFinder-n and log in:

<https://login.ezproxy.lib.umn.edu/login?url=https://scifinder-n.cas.org>

If you *do not yet* have a SciFinder account, go to <http://libguides.umn.edu/59310466> to register and then use your username and password combination to access SciFinder-n at <https://login.ezproxy.lib.umn.edu/login?url=https://scifinder-n.cas.org>.

To learn more about using SciFinder-n see:

- [Sci-Finder-n Quick-Start Guide](#)
- [SciFinder-n How-To videos](#)

Please contact Meghan Lafferty (mlaffert@umn.edu) with any questions.

Student Learning Outcomes (Some Obvious, Some Less Obvious):

In this course, you will

Identify, Define, and Solve a Range of Fundamental Problems in Chemistry – Physical chemistry permeates all aspects of chemistry. In this lab, we will address representative problems in kinetics, thermodynamics, and quantum mechanics, and will work with molecules as simple as HCl or as complex as 4-anilino-4'-nitroazobenzene. This will involve problems ranging from diffraction phenomena to the determination of bond lengths and potential energy surfaces, to the measurements of reaction rates and activation energies. The understanding of these experiments should enable you to address fundamental aspects of whatever phenomena your future interests lead you to.

Locate, Collect, and Analyze Data – Collecting and analyzing data is inherent in any laboratory course. The term “data” may be particularly relevant in a physical chemistry lab insofar as we will be making quantitative measurements and developing the sophistication needed to understand their meaning and limitations. An important part of this is error analysis, which will be an integral part of your lab write-ups, and which will be a topic we will address early in the semester. You will also be called upon, at times, to *locate* data in the chemical literature in order to compare your results with those of others. Sometimes this is easy, sometimes not so easy. Developing the skills to hunt down what you’re looking for in the vast chemical literature is something that will benefit any working chemist.

Demonstrate Fundamental and Predictive Knowledge of Chemistry – This Student Learning Outcome is realized largely through the fundamental theories that we will use to make and test predictions in the laboratory. Quantum mechanics, for example, is a remarkable predictive tool for anyone working with atoms and molecules. You will also have ample occasion to compare theoretical predictions against experimental data, an act which is, of course, fundamental to the scientific endeavor.

Acquire Skills for Effective Communication of Scientific Information – This is an important part of CHEM 4511W. See the discussion on page 2 under “Writing Intensive Course.”

OFFICE HOURS AND GETTING HELP

Instructor:

I will hold office hours weekly at the following times:

Monday 1:00 – 2:00
Thursday 2:30 – 3:30

I will also be available in lab to answer questions and/or make appointments for mutually convenient times. You can call (612-625-6072) or e-mail me (kleopold@umn.edu).

TAs will also be available. Connor Reilly and Luis Padilla will hold office hours at times to be announced. You can also ask questions via e-mail, and can usually expect a reply within a few hours (but not after 10:00 PM). Occasionally, a reply may take longer, but generally not more than 24 hours.

Due Dates:

Pre-lab assignments should be completed before you begin the lab experiment on any given week. The TAs will check that you have this done, and you won't be able to start the lab until you do. So please be sure to do these before coming to lab. These assignments exist in order to help you know what you're doing.

Lab reports will generally be due a little over two weeks from the date you do the lab. We want you to have time to do your best work and this will ensure that you have plenty of time, including two weekends. Note, however, that there are a few exceptions:

For the first few labs of the semester, we will be giving you opportunities to receive feedback on the lab reports. You will then be able to re-write the lab in order to (hopefully) get a better grade. This applies to the Diffraction Lab and either the HCl/DCI Lab OR the I₂ Fluorescence Lab (your choice). In order to get the most timely feedback, the initial version will be due only one week after the lab is done. Later in the semester, you will also have the option of rewriting either the Bomb Calorimetry or the Self Assembled Monolayer report.

PLEASE SEE THE SCHEDULE AT THE END OF THIS SYLLABUS FOR SPECIFIC DUE DATES.

Late Reports: *Please show consideration for the TAs by turning in your reports on time.* You will not be penalized for missing or delaying assignments due to a university approved activity or legitimate circumstance. For questions as to what counts as an approved or legitimate circumstance, see the university policy on make-up work on page 8. If an excused absence results in missing an experiment, a make-up experiment can be arranged during the semester. It is your responsibility to contact the TAs and instructor to schedule this time. Missing a lab report or a deadline without approval will result in 5% reduction in your score for that assignment per day (including weekends). Ideally, approval should be obtained before the missed lab or deadline. We recognize, however, that sometimes circumstances prohibit this, in which case please contact us as soon as possible.

Please Note: If you miss a lab, you must make up the lab. You cannot just get the data from your usual group. The reason is that this is a lab course, so doing lab work is central to the experience.

Also Note: In preparing your lab reports and worksheets, the work you submit **must be your own**. You may discuss your data or ideas related to it with other students, **but under no circumstances should text, tables, or figures be duplicated from others' reports**.

On the Use of Artificial Intelligence in This Course:

In the past year, open-source artificial intelligence (AI) (e.g., Chat GPT) has emerged as a powerful and rapidly evolving technology. It is “out there” and it is impossible to effectively forbid its use. However, like any technology, it has the potential to be used either wisely or unwisely, and it is therefore important to articulate the limits of its acceptable use in this course. **You may** use artificial intelligence, but only as an information-gathering tool. To be consistent with the goals of this course, the following rules apply:

- **You may not use AI to write your lab reports.** Remember: “Writing is Thinking”, and your depth of understanding will be far better if you have formulated ideas and assembled them into a logical progression on your own.
- Platforms such as Chat GPT sometimes get things wrong and, in some cases, even fabricate information. You are all within a few months of being card-carrying, credentialed chemists, and it is important to be right. **Fact check anything you dig up on Chat GPT.** Points will be deducted from lab reports for information that is clearly incorrect.
- Note that I have tested Chat GPT by asking it to provide text regarding topics covered in this course. The quality of the results is variable. Remember: artificial intelligence is not really intelligent. It is an algorithm that culls text from the vast database of the internet. Its writing is sometimes remarkably good, but it can also be sufficiently bland and repetitive in its style that its use becomes detectable to a trained reader.
- Submitting work generated by artificial intelligence while claiming it to be your own is a form of scholastic dishonesty and it will be treated as such. AI is not going away and many of you will likely use it in your future employment. Therefore, **it is important to develop a sense for how to use AI wisely and in a manner consistent with high standards of academic and personal integrity.**

You should, by all means, plan on getting assignments submitted on time. However, if circumstances occasionally conspire such that you're pressed for time before a deadline, please ask for an extension rather than use an AI shortcut to write your lab report.

We are all learning to adapt to the new reality that AI presents. I am happy to discuss any of this with you, either individually or as a group, so don't hesitate to ask!

Regrade Policy:

Questions about grading of lab reports should first be brought to the TAs. The reason is that they are in the best position to evaluate your concerns in the context of fair treatment to others. If a situation becomes unresolvable, then bring the issue to the instructor (K. Leopold). Again, please be

reasonable: We ask that if you have questions about a graded assignment, you bring it to the attention of the grader **within two weeks** of the date that the grade is posted. Inquiries beyond that time period will not be addressed.

Course Grades:

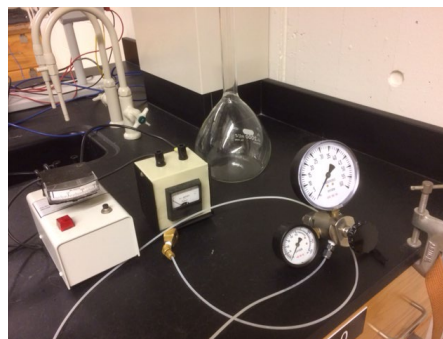
Although each lab will be performed in small groups (typically 3-4 people), the grading will be done on an individual basis and each assignment must be completed by each individual. Discussion of assignments including lab work, result, concepts, and analysis methods are highly encouraged. However, sharing data between groups and duplicating writing are strictly prohibited.

The final grade in the class will be assessed based on

- Lab reports (5 of them, 100 points each)
- Lab-based worksheets and assignments (5 of them, 50 points each, except for the fluorescence quenching report, which is a bit more involved and is worth 100 points.)

A final score will be calculated as the number of points obtained divided by the total number of possible points, quoted as a percentage. For labs that involve rewrites, only the higher grade will be counted. The final score will be used to assign letter grades according to the following rubric:

87 – 100	A
83 – 87	A–
80 – 83	B+
74 – 79	B
70 – 74	B–
66 – 70	C+
57 – 66	C
48 – 57	C–
43 – 48	D



If you happen to fall on one of the cusps, the higher grade will be assigned. Note that at the end of the semester, I may opt to adjust these cutoffs such that it will be possible to get a particular letter grade with a score that is lower than the range indicated above. But in no case will this adjustment hurt your grade. **That is to say, any adjustments, if applied, will only be used to improve your grade, not lower it.** However, you can use these as reasonable benchmarks to assess how you're doing in the course.

Incompletes:

The departmental policy on incompletes mainly addresses students who have to miss a final exam. Since we don't have a final exam, there will be few, if any, circumstances in which the requisite stipulation will apply. We will consider highly extenuating circumstances on a case-by-case basis. However, note that the following part of the departmental policy does apply:

Policy on Incomplete (I) grades:

The policy of the Chemistry Department is that a student may request an Incomplete grade only when (a) the student has a University sanctioned excuse for missing the final exam and (b) the student is passing the course based on all other graded components. Assignment of an I requires

that the instructor and student sign a contract, available in the Departmental undergraduate office, stipulating the procedure by which the I grade will be made up (e.g., taking a final exam from another instructor in the next semester). Failure to successfully complete the procedure outlined in the contract will result in the I being administratively changed by the University Registrar to an F or N (depending on the grade base) one semester (excluding summer) from the end of the semester for which the I grade was granted.

** Note that the University has policies already in place to permit students called to military service, or unexpectedly disabled by major medical issues, to petition for withdrawal (and potential full or partial tuition remission) without prejudice.*

Withdrawals:

We hope that you will successfully complete this course. If, however, it becomes necessary to withdraw from the course you must officially do so following the rules for your college.

Credits and Workload Expectations:

One credit is defined as equivalent to an average (over a full semester) of three hours of learning effort per week necessary for an average student to achieve an average grade in the course. For example, a student taking a three credit course that meets for three hours per week should expect to spend an additional six hours per week on coursework outside the classroom in order to achieve an average grade.

Policy on Scholastic Dishonesty:

Scholastic dishonesty is any conduct described as follows (from the "CLA Classroom Grading and Examinations Procedures"):

"Scholastic dishonesty is any act that violates the rights of another student with respect to academic work or that involves misrepresentation of a student's own work. Scholastic dishonesty includes (but is not limited to) cheating on assignments or examinations; plagiarizing (misrepresenting as one's own anything done by another); submitting the same or substantially similar papers for more than one course without consent of all instructors concerned; depriving another of necessary course materials; sabotaging another's work."

If a student engages in scholastic dishonesty, the instructor will at least assign a grade of zero on the work involved and will report the matter to the Office of Community Standards. An F in the course may also result. For more information on scholastic dishonesty, see

http://regents.umn.edu/sites/default/files/policies/Student_Conduct_Code.pdf

If in doubt as to whether or not an action constitutes scholastic dishonesty, please feel free to ask me. I will welcome the discussion.

Policy on Appropriate Use of Course Materials:

Taking notes is a means of recording information and of personally absorbing and integrating the educational experience. However, broadly disseminating class notes or exams beyond the classroom community or accepting compensation for taking and distributing such items undermines instructor interests. **This means "Don't upload course materials (including your lab reports) to sites like**

Chegg, Course Hero, etc.). Engaging in such actions violates shared norms and standards of the academic community and now carries consequences in the Offices of Community Standards. It is unethical, so please don't do it.

Students with Disabilities:

We are happy to accommodate students with disabilities. Please work with the Disability Resource Center (612-626-1333), where you can get a letter outlining what would be the most appropriate accommodations for you. Once you have that, please contact the instructor to work out details of how to implement those accommodations.

Lab Atmosphere:

Lab work in this class is done in a group environment, and it is important that everyone be allowed to contribute both to performing the labs and to developing the intellectual interpretation of the results. Harassment and behavior that excludes students from full participation will not be tolerated. The University will provide 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.

We will gladly honor your request to address you by an alternate name or gender pronoun. Please advise us via email or in person at the beginning of the semester so that the teaching assistants and I can address you properly in or outside of class.

For more information, refer to the University policies listed below:

University of Minnesota, Mental Health Services Syllabus Statement:

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 or reduce a student's ability to participate in daily activities. University of Minnesota services are available to assist you with addressing these and other concerns you may be experiencing. You can learn more about the broad range of confidential mental health services available on campus via the Student Mental Health Website at <http://www.mentalhealth.umn.edu>

Additional Policies Pertinent to Classes at the U of M (and this course as well):

Board of Regents Policy on Equity and Diversity:

http://regents.umn.edu/sites/default/files/policies/Equity_Diversity_EO_AA.pdf.

Student Conduct Code:

http://regents.umn.edu/sites/default/files/policies/Student_Conduct_Code.pdf

Sexual Harassment:

https://regents.umn.edu/sites/regents.umn.edu/files/policies/Sexual_Harassment_Sexual_Assault_Stalking_Relationship_Violence.pdf

Makeup Work for Legitimate Absences:

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

Use of Personal Electronic Devices in the Classroom:

See statement in <http://policy.umn.edu/education/studentresp>

Appropriate Student Use of Class Notes and Course Materials

<http://policy.umn.edu/education/studentresp>

Grading and Transcripts:

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

Disability Services:

<https://regents.umn.edu/sites/regents.umn.edu/files/policies/DisabilityServices.pdf>

Academic Freedom and Responsibility:

See statement at <https://policy.umn.edu/education/syllabusrequirements-appa>

CHEM 4511W SCHEDULE – Fall, 2023

<u>Week</u>	<u>Monday Lecture Topics</u> (Subject to Changes, As Needed)	<u>Tuesday/Wednesday (Lab)</u>	<u>What's Due This Week?*</u> Unless Otherwise Noted, All Assignments are due on: Wednesday, 11:59 PM for the Tues. Section or Thursday, 11:59 PM for the Wed. Section
1 9/5 - 9/8	No Class (Labor Day)	Meet in 465 Kolthoff; Discuss Course/Syllabus; Group Assignments T, 9/5 or W, 9/6	Read chapters 1 and 2 of lab manual by lab day next week.
2 9/11- 9/15	M, 9/11 * Diffraction Lab Prep. * Error Analysis * Begin Scientific Writing, (as time permits)	*Diffraction Lab (Light and Electrons)	*Read the Computational Chemistry handout by lab day next week
3 9/18 - 9/22	M, 9/18 *Scientific Writing: Data Presentation, Formatting, Full Report	* Hydrogen Spectrum & * Computational Chemistry (Done in the Microlab, 101 D, Smith Hall)	*Error Analysis Worksheet Due MONDAY, 9/18 (both sections) *Experimental and Results sections for the Diffraction lab: T Sec: 9/20 at 11:59 PM W Sec: 9/21 at 11:59 PM
4 9/25 – 9/29	M, 9/25 * Finish Scientific Writing * HCl/DCI Lab Prep.	* HCl/DCI IR Spectrum	*Diffraction Lab Full Report T Sec: 9/27 at 11:59 PM W Sec: 9/28 at 11:59 PM
5 10/2 - 10/6	M, 10/2 *I ₂ Fluorescence Prep.	I ₂ Fluorescence Lab	*Computational Chemistry Worksheet *Hydrogen Worksheet T Sec: 10/4 at 11:59 PM W Sec: 10/5 at 11:59 PM *Diffraction Lab Rewrite T Sec: 10/6 at 11:59 PM W Sec: 10/7 at 11:59 PM Note irregular due date here.
6 10/9 - 10/13	M, 10/9 *Rotating Labs – Prep. Part I	BREATHING WEEK NO LAB ☺	* HCl/DCI Lab Report T Sec: 10/11 at 11:59 PM W Sec: 10/12 at 11:59 PM

7 10/16 - 10/20	M, 10/16 Rotating Labs – Prep. Part II	Rotating Labs – 1 (Thermo and Kinetics)	*I ₂ Fluorescence Lab Report T Sec: 10/18 at 11:59 PM W Sec: 10/19 at 11:59 PM
8 10/23 - 10/27		Rotating Labs – 2 (Thermo and Kinetics)	*Rewrite of either HCl/DCI or I ₂ Fluorescence Lab T Sec: 10/25 at 11:59 PM W Sec: 10/26 at 11:59 PM
9 10/30 - 11/3		Rotating Labs – 3 (Thermo and Kinetics)	*Lab Report from Week 7 T Sec: 11/1 at 11:59 PM W Sec: 11/2 at 11:59 PM
10 11/6 - 11/10		Rotating Labs – 4 (Thermo and Kinetics)	*Lab Report from Week 8 T Sec: 11/8 at 11:59 PM W Sec: 11/9 at 11:59 PM
11 11/13 - 11/17		NO LAB THIS WEEK ☺	*Lab Report from Week 9 T Sec: 11/15 at 11:59 PM W Sec: 11/16 at 11:59 PM
12 11/20 - 11/24		Thanksgiving Week – No Lab	
13 11/27 – 12/1		NO LAB THIS WEEK ☺	*Lab Report from Week 10 T Sec: 11/29 at 11:59 PM W Sec: 11/30 at 11:59 PM
14 12/4 - 12/8		NO LAB THIS WEEK ☺	*Re-write of ONE Rotating Lab Report (Calorimetry or Monolayers) T Sec: 12/6 at 11:59 PM W Sec: 12/7 at 11:59 PM
15 12/11 - 12/13		NO LAB THIS WEEK ☺	

*This column does not explicitly give due dates for reading the week's lab or doing the pre-lab assignment. You are always expected to do this prior to coming to lab. Remember that the "lab report" for the Hydrogen Atom Spectrum, Fluorescence Quenching, and Isomerization Kinetics labs are really worksheets.