CHM4411L: Physical Chemistry Laboratory

Spring 2025 2 credit hours

Class Number(section): 18890(PL1T), 10609(PL1W), 10610(PL1R), 25678(PL1F)

M Period 5 (11:45 - 12:35) LEI 242 ; T W R F 6-10 (12:55-18:00) LEI 248

No (specifically) Required Textbook: Notes for this course will be provided online; Complete understanding of the activities will require external resources to be sourced by the individual. It is assumed that you have access to a typical Physical Chemistry textbook, such as the one used in CHM4411 and/or CHM4412.

Contact Brucat if you have questions...

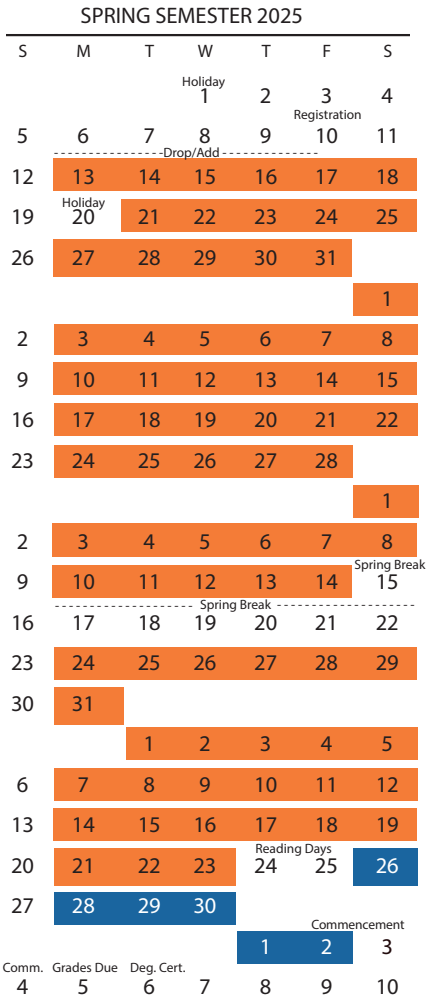
Instructor: PJ Brucat

- Office hours (subject to optimization):
  Monday 12:50 - 13:40
  Friday 10:40 - 11:30
  or by appointment (message three choices)
- Contact method: *Canvas Messaging only*. No Email.

TA: Yiheng Yan
Ignacio Pickering

Course Website:
https://ufl.instructure.com/courses/

All communication and activities related to this course will be accessible from within UF's campus-wide eLearning system (Canvas) at the URL above. Please become familiar with our course website as soon as possible. Much of the materials there are be subject to revision, so pay careful attention to all announcements, updates, and revision dates. *It is strongly advised that hardcopy or static downloads of course materials be avoided due to their continuous incremental improvement.*



Deportment

Your polite, courteous, and civilized behavior is expected in all aspects of our course. Be Human. Be good to each other. Smile. Embrace a spirit of exploration, community, and positivity.

Recordings

State law permits unregulated, unannounced audio and/or video recording of all aspects of course meetings without prior consent. Therefore, participants in this course should assume that they are being recorded at any time during class meetings.

Goals and Objectives

Course Goals

The purpose of this course is to augment, reinforce, and complement the concepts and topics covered in the CHM4411 "Thermodynamics and Kinetics" and CHM4412 "Quantum Mechanics and Spectroscopy" lecture courses.

Successful completion of this course will enable the learner to:

- Apply the Scientific Method to the investigation of the natural world.
- Synthesize the concepts of Quantum Mechanics, Spectroscopy, and Statistical Mechanics into testable hypotheses.
- Master the basic concepts of experimental design.
- Develop a working understanding of computer programming for experimental control, data acquisition, data visualization and data analysis.
- Master the concise and effective communication of scientific observations and conclusions.

Course Objectives

Accomplishment in the course material will be assessed in the following:

Knowledge

- Statistical methods in extracting model parameters from quantitative observation
- Basic elements of scientific programming with Python in a Jupyter environment
- Clear and cogent rendering of scientific observations in the format expected of peer-reviewed scientific publications
- Professional short-form reporting of scientific activity

Skills

- Collection and manipulation of data
- Creation of publication-quality figures
- Authoring high-quality short reports/executive summaries

Lab Etiquette

A laboratory space is special in many ways. Not only does it contain an array of strange and wonderful objects, it has unusual dangers and concerns. A teaching laboratory has an additional layer of behavioral constraints, as it is, by necessity, occupied by individuals not specialists (yet) in the purpose and function of the equipment therein. Moreover, such a lab space is *shared* by many, and therefore all occupants are *guests* and need to heed the criteria for being a *good guest*.

That said, what makes a good guest? Think about how you would behave if you were staying at a respected friend's house.

- Don't go nosing into drawers or touching things that you have not been given permission to use.
- Clean up after yourself. You do not have maid or nanny in the lab. You make a mess, you clean it up. Leave everything as good or better than you found it.
- Don't hesitate to ask for instruction/permission to use something *before* you use it.
- Report anything you break or find broken.
- Act in a *professional manner*. See the Professional Behavior expectations under Grades.

Course Operation

Course Meetings

There are two meeting types intrinsic to the learning experience of this course.

1. **Lectures** This course has regularly-scheduled meeting times designated for synchronous meetings of the entire class. These meetings are a one-on-many environment primarily for discussion and explanation of new material outlined in the course Attendance at these meetings is *required*. UF attendance policies are in effect. If you fail to absorb information from these discussions, you will have difficulty completing the laboratory challenges and/or submitting quality assignments. Moreover, you may be a burden to your lab partner and unsafe and a risk to everyone. Attend lecture.

2. **Laboratory Sessions** The actual experimentation will take place in the PChem Teaching Laboratory, LEI 248. It should go without saying that physical attendance in the lab session is *required*. If you are unable to attend the lab session, notify the instructor as soon as possible prior to that session. If the absence is allowable by University policy https://catalog.ufl.edu/UGRD/academic-regulations/attendance-policies/, a makeup session will be arranged. No grade points will be awarded for any assignment associated with a session you did not attend.

Communication with your Instructor

To guarantee rapid, reliable, and secure transmission, all course communications with your instructor(s) are to occur within the Canvas environment using the embedded tools. Configure your Canvas account profile for immediate automatic notification of course announcements and updates, and make sure that email forwarding, if desired, is set up correctly. It is expected that all replies to messages between instructor and student occur within 24 hours.

To request a meeting with your instructor, send three time choices convenient to you via Canvas messaging to whom you wish to meet. Your instructor will respond by choosing one of those times with a location. This process minimized the complexity of *ad hoc* meeting scheduling and is a required protocol. Meeting requests that do not contain at least three time choices will be ignored. Responsibility for receiving and responding to electronic course communication in a timely fashion is entirely that of the student.

Groups

Laboratory activities will be undertaken in groups of two. Your group designation will determine the laboratory activity schedule. Group assignments may be found in the course Canvas website.

You are expected to work professionally and efficiently with your group partner. Troublesome partnerships will suffer from Professional Behavior grades.

All graded assignments will be be worked and submitted as *individuals*. Clearly, data sharing and other collaboration is expected between the group members, but outright *copying* any portion of an assignment submission is *not allowed*. Assignment submissions are to be your *own original work*. Plagiarism in any way is a violation of UF's Honor Code.

Graded Assignments

Analysis Quizzes (AQ)

For most lab activities, a short question set will be delivered online through our course website. These quizzes are intended to be *formative* assessments, in that these activities focus on and cement concepts in the learner's mind related to the experiment performed that week. These quizzes are entirely based on material relevant to the analysis and interpretation of your observations, and should be helpful in the crafting of your ES report, *vide infra*. Any non-sentient resources may be used to solve these quiz problems, as long as they are worked entirely individually, without consultation with anyone except your instructor(s). To repeat: You may discuss the quiz *only with your instructor(s)* until after the due date has passed for everyone in the class.

Python/Jupyter Notebook (NB)

Data visualization and quantitative analysis is key to any experiment, and the Scientific Method in general. The Jupyter notebook environment, running a Python3 kernel, will be used for processing the numerical results of the guided inquiries of the lab. No, Excel or other spreadsheet programs will not be sufficient for the manipulation and rendering of data in this course. Students will submit Python notebooks to our class Jupyter server as part of their reporting. Fear not. No prior programming experience is necessary to master the creation and use of these notebooks. Extensive hints and templates will be provided.

Executive Summary (ES)

After some lab sessions you will be asked to report your observations. This will be in the form of an *Executive Summary* of the hypotheses, procedures, findings, and conclusions. Some form of data analysis and graphical representation, usually in the form of publication-quality captioned figures will be required. The ES is a shorter, more focused, and less formal than a typical journal publication. Specific requirements and guidelines for each ES will be provided in the activity description.

Each ES will be submitted to the appropriate Canvas assignment page the format requested for grading. Some materials may be need to be authored on or uploaded to the class Jupyter server. These may be referenced in the ES document but not uploaded to the assignment page. Submissions not in the required format will be ignored and generate no grade points.

Laboratory Activity Schedule **(Tentative; see course website)**

Week	Date	Lecture	Group ID			
			G1	G2	G3	G4
1	01/13	01	–	–	–	–
2	01/20	–	PDA	PDA	PDA	PDA
3	01/27	02	PDB	PDB	PDB	PDB
4	02/03	03	HA	HA	HA	HA
5	02/10	04	PC	PC	PC	PC
6	02/17	05	AS	AS	AS	AS
7	02/24	06	IR	LF	IR	LF
8	03/03	07	LF	IR	LF	IR
9	03/10	08	NMRA1	EPR1	NRA2	EPR2
10	-	–	-	-	-	-
11	03/24	09	EPR2	NRA2	EPR1	NMRA1
12	03/31	10	NMRB1	PK	NMRB2	PK
13	04/07	11	PK	NMRB1	PK	NMRB2
14	04/14	12	MUW	MUW	MUW	MUW
15	04/21	–	-	-	-	-

PDA is 'Plotting Data A', an introduction to Jupyter/Python and data visualization and regression.

PDB is 'Plotting Data B', continued activities using Jupyter/Python for data analysis and spectral decomposition.

HA is 'Hydrogen Atom Spectrum', the analysis of the emission spectrum of a Hydrogen discharge lamp.

PC is 'Determination of Planck's Constant', a quantitative study of the emission wavelength and forward bias voltage of LED devices of various bandgaps.

AS is 'Acoustic Spectroscopy', A study of impulse response and swept frequency methods in spectroscpy, using audio frequencies and sound.

IR is 'Infra-Red Spectra of Greenhouse Gases', the spectroscopic study of IR absorption in various gases.

LF is 'Laser Induced Fluorescence in I_2 Vapor', the analysis of optical emission of laser-excited Iodine vapor.

NMRA* is 'Nuclear Magnetic Resonance (A)' is a study of a driven two-level spin system and the observation of Rabi nutation. The session will be split into two time slots: NMRA1 session starts at 13:15. NMRA2 session starts at 15:15.

EPR* is 'Electron Paramagnetic Resonance' is a study of the electron spin in open-shell systems. The session will be split into two time slots: EPR1 session starts at 13:15. EPR2 session starts at 15:15.

NMRB* is 'Nuclear Magnetic Resonance (B)' is a study of longitudinal and transverse relaxation. The session will be split into two time slots: NMRB1 session starts at 13:15. NMRB2 session starts at 15:15.

PK is 'Photolysis Kinetics', a study of the reversible photoisomerization of azobenzene.

MUW is a makeup week. Activities scheduled *ad hoc*

Assignment Schedule **(Tentative; see course website)**

Week	AQ	Due	NB	Due	ES	Due
1	SYLQ	01/15				
2	SAFQ	01/22	NB-PDA	SD+1		
3			NB-PDB	SD+1		
4	AQHA	02/07	NB-HA	SD+1	ES-HA	SD+3
5	AQPC	02/14			ES-PC	SD+3
6	AQAS	02/21			ES-AS	SD+3
7-8	AQIR	SD+2	NB-IR	SD+3		
7-8	AQLF	SD+2			ES-LF	SD+3
9-11	AQNMR	SDA+2			ES-NMRA	SD+3
10	—	—	*Spring*	*Break*	—	—
9-11	AQEPR	SD+2			ES-EPR	SD+3
12-13					ES-NRMB	SD+3
12-13	AQPK	SD+2	NB-PK	SD+3		
14	MUW		MUW		MUW	
15						

SYLQ is the Syllabus Quiz.

NB-* are a Jupyter/Python notebooks submitted via our class Jupyter server. They are the backbone of the data analysis and visualization for all the activities in the course. In most cases hints and templates will be provided. No previous Python or programming experience is required.

SAFQ is the Safety Quiz. It is based on the materials found on the Resources page under Safety and Waste Management. Stay safe, my friends.

AQ-* are Analysis Quizzes.

ES-* are the Executive Summary reports.

SD+n are due dates for labs in rotation. The n indicates the number of days after the session date the assignment is due. See Canvas calendar for due dates specific for your rotation group.

Weeks 7-8, 9-11 and 12-13 are activity rotation periods. Exact assignments depend on Group.

All 'official' activity dates and grades are posted on the secure course website. Assignments are to be submitted in full by the assignment deadline in the requested format for credit.

Course Resources

· · · Activity Descriptions

Notes guiding and describing course activities are posted on the course website. The expectation is that these notes guide your preparation prior to attending the lab meetings. It is not expected that these notes will be sufficient on their own — This laboratory relies heavily on all the Chemistry that you have learned up to this time, and in particular, your Physical and Analytical Chemistry preparation. These activity descritons are subject of constant revision, so make sure you are using the latest version. For that reason, static downloads of the material are discouraged.

· · · The Course Jupyter Server

The majority of scientific data processing, data mining, and AI research relies on the computing 'language' Python. It is ubiquitous in Chemistry and has lots of community support around the globe. There are libraries (packages) for almost everything a Chemist wants to do already written in Python, so it is an obvious choice for a student of Chemistry. Moreover, Python is easy to learn. The internet provides multiple tutorials and helpful hints for almost any imaginable task in Python. Python can be used in an interactive development environment, Jupyter, which breaks up the commands into 'cells' which are executed in a flexible order. Jupyter has many of the features and behavior of other powerful apps like *Mathematica* or *MATLAB*, but is free, has huge support among Chemists, and has a shallower learning curve. Familiarity with Python in some form may just be what it takes to get you the job you want and the career you choose.

Graded data analysis and visualization assignments in this course will use a server spun up specifically for us. This Chemistry Department Jupyter server can be found here: https://jupyter2.chem.ufl.edu. Login there with your Gatorlink username (the part of your @ufl.edu email address before the @ symbol). The initial password you choose will be set for subsquent logins, so remember it. You may choose any password, but it is advised not to reuse a password from any other system. Note: If you are off campus, you must VPN into the UF network before hitting the server login page. Instructions for using VPN are on UF's website https://it.clas.ufl.edu/kb/category/vpn.

· · · Notebook Hints

To assist mastery of data processing and manipulation, detailed Python notebook 'hints' will be provided for each activity. These are not meant to represent the unique solution to the posed problem, but provide example code for scrutiny and modification. These 'hints' will be placed in the course webpage.

Grades

Course Grade Computation

Course grades will be computed from the weighted-average of the earned percentages of each graded items described under Course Activities, submitted by the individual student. The weighting factors of the activity categories are as follows:

Default Category Weights

Grade Category	weight %
Analysis Quiz (AQ)	20
Jupyter/Python Notebook (NB)	20
Executive Summary (ES)	40
Professional Behavior (PB)	20

The grading scheme will generate a aggregate assignment percentage, which will be converted into a letter grade as follows:

Course Letter Grade Percentages

Grade	A	A−	B+	B	B−	C+	C	D	E
Minimum percentage	87.5	80.0	77.5	72.5	70.0	67.5	60.0	50.0	< 50.0

Professional Behavior

Students in the advanced Physical Chemistry laboratory have mastered general, organic, and analytical chemistry laboratory material and procedures as a requirement. Therefore, high standards of accomplishment and maturity are expected in all aspects of student deportment. To be clear, students are expect at all times to act in a professional manner and behave as a skilled and experienced Chemist.

To be explicit, all essential aspects of professional behavior are required of the student and compliance with these criteria will be graded.

Essential elements of Professional Behavior include, but are not limited to:

- Record Keeping: All experimenters are expected to keep a complete and accurate notebook.
- Preparation: Before any lab session, all reading material relevant to the activity must be thoroughly studied and researched. Plans for the execution of the experiment should already be in place. Such plans should be documented in the student's individual notebook. Plans may be discussed and modified by the workgroup at any time, but each student should have a draft proposal for discussion at the initiation of experimentation.
- Safety: Experimenters are to understand follow all appropriate safety procedures.
- Cooperativity: Students are expected to follow instructions from instructors.
- Respect: All participants are expected to respect each other, their instructors, the equipment, the lab space, and institution of learning in which they are a member. This includes adherence to the aforementioned lab etiquette guidelines.
- Focus: Students are expected to be trained observers, focusing on the experiments they are performing and sensitive to any aberrations or unexpected phenomena. Surfing the web, playing games, or socializing while performing an experiment are obvious signs of lack of focus and are unprofessional.

Noncompliance with any feature of professional behavior will result in a severe grade penalty or complete zeroing of the grade category. Exemplary professional behavior is *expected*. Feedback will be provided if any indication of unprofessional activity is detected.

The professional behavior grade will be posted at the end of the term.

Regrade Requests

Grade accuracy is a high priority for this course. Assignments will be regraded if a grading error is suspected. Regrade requests from students must be submitted through Canvas Messaging to Brucat within 48 hours of the grade post. Regrades will be performed on the entire assignment following the standard assignment rubric. Grade adjustments may be positive or negative.

UF's Grading Policy

See https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

Student Resources

The best place to find all resources available to UF students in a wide range of topics, including mental and physical health, advice on academic and financial matters, violence prevention and more, is: https://one.uf.edu/whole-gator/discover

Specific resources, somewhat redundant to the above, are included below, for completeness.

Honesty and Truthfulness

Ethical, moral, and professional behavior is expected and required of all participants in this course. Moreover, all participants in UF's Academic activities are bound by Rules of Conduct, from which can be found the following excerpt:
"UF students are bound by The Honor Pledge which states,
'We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code.'
On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied:
'On my honor, I have neither given nor received unauthorized aid in doing this assignment'
The Honor Code (http://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class"

Additional Information

Accommodations

The Disability Resource Center at UF offers this advice:

"Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the Disability Resource Center by visiting our Get Started page. It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester."

Counseling

Useful non-academic services are available in many forms at UF.

- U Matter, We Care: If you or a friend is in distress, please contact umatter@ufl.edu or 352 392-1575 so that a team member can reach out to the student.
- The Counseling and Wellness Center: http://www.counseling.ufl.edu/cwc/

GatorEvals

The UF course evaluation policy includes the following statement:

"Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at https://gatorevals.aa.ufl.edu/students/. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via https://ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/."

All course policies and procedures are subject to change at any time at the sole discretion of Brucat

We, the members of the University of Florida Community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity

— Revision: January 7, 2025 —