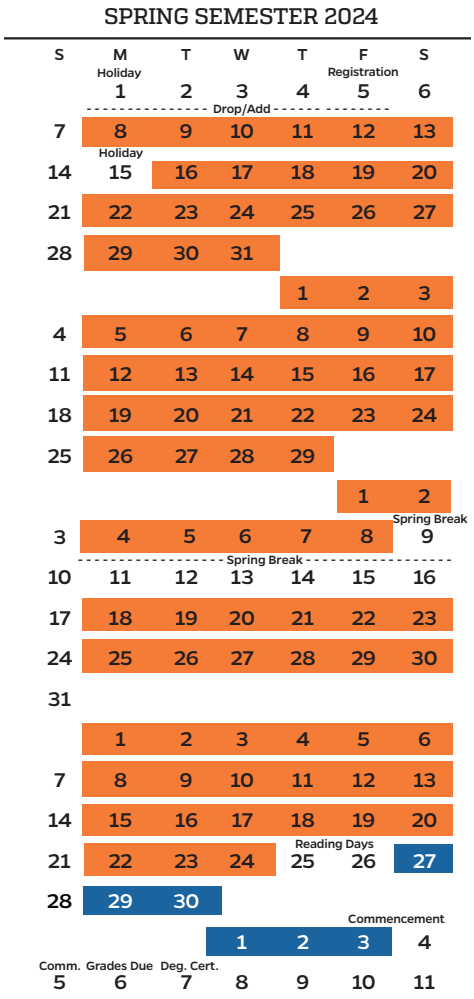
CHM4411L: Physical Chemistry Laboratory

Spring 2024 2 credit hours

Class Number(section): 25339(P3LM)

M Periods 5 (11:45 - 12:35) LEI 242 ; 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):
  TBA
  TBA
  or by appointment (message three choices)
- Contact method: *Canvas Messaging only*. No Email.

TA: TBA

Course Website:

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

All communication and activities related to this course will be accessible from within UFs 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.*

Etiquette

Your polite, courteous, and civilized behavior is expected in all aspects of our course. This holds especially true in these times of stress and uncertainty. Be Human. Be good to each other. Smile.

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

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.

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. 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 poor subjective 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 copying assignment submissions or other is not allowed. Assignment submission 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 each lab activity, short question sets will be delivered online through our course website. These are intended to be *formative* assessments, in that these activities focus on and cement concepts in the learner's mind. 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 resources may be used to solve these quiz problems, as long as they are worked entirely individually, without consultation with anyone except your instructors. You may discuss the quiz *only with your instructors* 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. 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 each lab session 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.

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. Submissions not in the format requested will be ignored.

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

Week	Date	Lecture	Group ID			
			G1	G2	G3	G4
1	01/08	01	PDA	PDA	PDA	PDA
2	01/15	–	–	–	–	–
3	01/22	02	PDB	PDB	PDB	PDB
4	01/29	03	HA	HA	HA	HA
5	02/05	04	PC	PC	PC	PC
6	02/12	05	IR	LF	IR	LF
7	02/19	06	LF	IR	LF	IR
8	02/26	08	PKA	PKA	PKA	PKA
9	03/04	09	PKB	PKB	PKB	PKB
10	-	–	-	-	-	-
11	03/18	10	PT	PT	PT	PT
12	03/25	11	NMR1	EPR1	NMR2	EPR2
13	04/01	12	EPR2	NMR2	EPR1	NMR1
14	04/08	13	QC	QC	QC	QC
15	04/15	–	MUW	MUW	MUW	MUW

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.

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

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

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.

PT is 'Passive Transport', a study of the migration of ions through a membrane as a result of a concentration gradient.

PK* is 'Photolysis Kinetics', a study of the reversible photophysics of azobenzene. This is a two session activity (A and B) which will include a draft and final report, as well as a quiz.

QC is 'Quantum Chemistry', a study computational study of the electronic structure of small molecules.

NMR* is 'Nuclear Magnetic Resonance: Basic Physics' is a study of nutation, FID, and relaxation in proton magnetic resonance. NMR1 session starts at 13:00. NMR2 session starts at 15:00.

EPR* is 'Electron Paramagnetic Resonance' is a study of the electron spin in open-shell systems. EPR1 session starts at 13:00. EPR2 session starts at 15:00.

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

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

Week	AQ	Due	NB	Due	ES	Due
1	SYLQ	01/12	NB-PDA	01/15		
2	SAFQ	01/17				
3			NB-PDB	01/24		
4	AQHA	02/01	NB-HA	01/31	ES-HA	02/02
5	AQPC	02/08	NB-PC	02/07	ES-PC	02/09
6	AQIR	SD+3	NB-IR	SD+1	ES-IR	SD+5
7	AQLF	SD+3	NB-LF	SD+1	ES-LF	SD+5
8	AQPK	02/28	NB-PKA	02/29		
9					ES-PKB	03/08
10	—	—	*Spring*	*Break*	—	—
11	AQPT	03/20			ES-PT	03/22
12	AQNMR	SD+3	NB-NMR	SD+5		
13	AQEPR	SD+3			ES-EPR	SD+5
14					ES-QC	04/12
15	MUW	04/17	MUW	04/18	MUW	04/19

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. They precede every experiment with a review of concepts and computations.

ES-* are the Executive Summary reports. These are concise, cogent reports meant to summarize the activity and describe the results and conclusions to an educated expert, but one unfamiliar with the specific activity. All executive summaries include publication-quality figures which represent the type and quality of the data obtained by the experimenter as well as a quantitative graphical comparison of the observation and hypotheses posed by the experimenter.

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 5-6 and 12-13 are activity rotation periods. Exact assignment dates depend on Group. See Canvas site for details.

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 in all the courses you have taken thus far, and in particular *CHM4411 Thermodynamics and Kinetics*. The lab notes are subject of constant revision, so make sure you are using the latest copy. 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 a job.

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://jupyter.chem.ufl.edu:8000/. Login there with your Gatorlink username (the part of your @ufl.edu email address before the @ symbol) and the initial password 'mechanicup'. Instructions for changing your password to protect your work will be provided in our first meeting. You must change your password to protect your work. 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.

It is also strongly encouraged that you install Python on your own devices, if it is not already. '*Anaconda*' is a free code suite that allows one to easily setup Jupyter/iPython/R on your personal devices. Free download and instructions can be found on the website: https://www.anaconda.com/distribution/. Anaconda is also available through UF apps (https://apps.ufl.edu) for all UF students. My experience with UFapps is mixed, and I cannot recommend it except for casual use.

··· 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 your workspace on the course Jupyter server or on the course website.

··· HiPerGator

UF has a large, world-class, high-performance computing facility used for research computing. Enrollment in this course will provide you temporary access to that environment. HiPerGator will be used for some example Quantum-Chemical calculations relevant to course activities, and some of the fundamentals of AI/ML will be demonstrated if time permits. Details are to be found on the eLearning resources page.

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
Instructor Subjective (IS)	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

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

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"

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: December 28, 2023—