CHM4411:
Thermodynamics
(with Kinetics, Transport, and Statistical Mechanics)

Fall 2024 4 credit hours

Class Number(section): 23892(P410)
M W Periods 2-3 (08:30 - 10:25) LEI 242

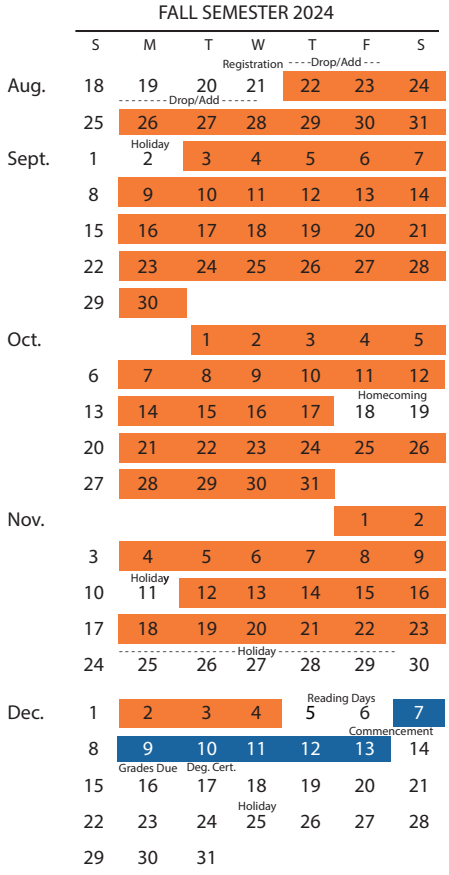
No (specifically) Required Textbook:
Useful texts include *the one you have* or something like:
"Physical Chemistry", P. W. Atkins *et. al.*, any addition, or similar titles by McQuarrie & Simon, Levine, Raff, Castellan
Notes for this course will be provided online, however, you *need* a at least one textbook. Multiple sources and perspectives will augment your breadth of understanding.

Contact Brucat if you have questions...

Instructor: PJ Brucat
- Office hours (subject to optimization):
  Mon 10:30-11:30 ; Fri 08:30-09:30
  or by appointment (message three choices)
- Contact method: *Canvas Messaging only*

TA: TBA

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. Pay careful attention to all announcements, updates, and revision dates. *Hardcopy or static downloads of course materials are strongly discouraged* as these resources are subject to continuous incremental improvement.



Etiquette

Your polite, courteous, and civilized behavior is expected in all aspects of our course. Be kind to each other. Be Human.

Recordings

State law permits unregulated, unannounced audio and/or video recording of all aspects of course meetings without prior consent 'for personal use', whatever that means. Therefore, all participants should assume that they are being recorded at all times.

Goals and Objectives

Course Goals

Successful completion of this course will enable the student to:

- Integrate the Scientific Method into the Investigation of the Natural World
- Apply the Postulates and Methods of Thermodynamics to Chemical Systems
- Develop Models to Simulate the Time-Dependence of Macroscopic Systems
- Statistical Methods to the Interpretation of Ensemble Properties
- Program Computational Tools for Symbolic and Numerical Solutions to Chemical Problems

Course Objectives

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

Knowledge

- Guiding Principles of Thermodynamics
- Kinetic Models
- Transport Models
- Ensembles
- Statistical Methods

Skills

- Use of Computational Tools in the Solution of Complex Chemical Problems
- Application of Thermodynamics to Chemical and Phase Equilibria
- Application of Thermodynamics to Electrochemistry
- Application of Numerical Methods to Chemical Kinetics
- Application of Counting Statistics to Statistical Thermodynamics

Course Operation

Course Meetings

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

1. **Scheduled Class Meetings** 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 in these meetings is *strongle recommended*. Meetings will not be recorded. The complete discussion outline (course notes) for each meeting will be posted to VoiceThread as part of the Community Review assignment. Community Review assignments are *not optional* and are graded. See Community Review
2. **Scheduled Office Hours** The purpose of regularly-scheduled 'office hours' is primarily to assist students as individually as possible in their specific learning needs. It is sometimes a one-on-one activity, but often the collective questions of a few like-minded students can be even more profitable. These activities are optional, but recommended if a learner finds themselves 'stuck' or frustrated in their advancement. Assistance and 'hints' towards the completion of the classwork and quizzes is also available here. Experience has shown that greater utilization of office hours is made when they are online, so this will be an option. See the Canvas Calendar for the schedule.

3. ***Ad Hoc* Conferences** Any student may request an *ad hoc* one-on-one meeting with the instructor, for whatever purpose, at any time. Such requests will be made exclusively through Canvas Messaging. Requests must include three distinct times for the requested meeting in the initial message and whether the meeting is desired to be private or open to other students, face-to-face or virtual. The Instructor will respond to the request within 12 hours (usually much less) by accepting one of the times and provide a video conferencing link or physical location for the meeting. Such conferences are not restricted to normal business hours, but may be constrained by conflicts with other meetings, health concerns, and mundane extraneous commitments.

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.

Course Activities

Synchronous Discussion

Twice a week, the entire class will meet for two hours to discuss Thermodynamics, Transport Phenomena, and Statistical Mechanics. These meetings are the core of the course, at least as far as the traditional definition of the University curriculum goes. To optimize your time and learning, these class discussions should involve active participation, which, in turn, requires individual preparation and review:

- Preparation For a discussion among a learning community to be profitable, preparation and a common reference must exist. Before every class meeting, the material to be covered that session (see Meeting Schedule) will be reviewed by careful reading of the course notes as well as aggregation of any additional material needed by the individual learner. It is highly recommended that each student keep a detailed notebook which should include documentation and details of the learning process. Any questions or comments that arise in the preparation period should be recorded in the notebook and brought to the class meeting.
- Participation At the start of every scheduled class meeting, a focussed discussion of the concepts covered in the previous session as well as a preliminary overview of the reading and scheduled session content. This disussion in part of your learning process, and aprticipation in this discussion is mandatory and graded. Participation is as much asking (non-trivial) questions as answering them. Participation is not annonymous. Participation credit cannot be assigned to absent learners.

Office Hours

Every student of Physical Chemistry is unique. The classwide discussions of the topics are necessarily a compromise, in that your instructor must target the group collectively, and thus imperfectly. It is expected *and encouraged* that each student take advantage of individual meetings with the instructor.

Formative Assessments

Physical Chemistry is a journey; Mastery of it is the goal. Progress is made towards mastery through activities that challenge and focus thinking and require application of what has been learned. There

will be three types of these activities:

Concept Quizzes (CQ) Periodically throughout the term (weekly, for the most part), 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 learners mind. These quizzes are entirely based on material in the course notes and are to be **worked individually**. That means you may **only discuss the quiz and its contents with your instructor** until after the due date.

Course Work (CW) Class Work is a set of exemplary problems to challenge your skill and cement your mastery of the material. These are approached by the individual student asynchronously. Collaboration is allowed and encouraged. However, each student must **submit their own individual work** for grading by the instructor. Submitting someone else's work as your own not only impedes the instructors ability to assist your learning, but is also a violation of the Honor Code.

Class Participation (CP)

Assignment Schedule

(tentative; see Canvas website course stream)

Week	Assigment	Due Date	Assignment	Due Date
0				
1	CQ00	08/27	CW00	08/30
2	CQ01	09/03	CW01	09/06
3	CQ02	09/10	CW02	09/13
4	CQ03	09/17	CW03	09/20
5	CQ04	09/24	CW04	09/27
6	CQ05	10/01	CW05	10/04
7	CQ06	10/08	CW06	10/11
8	CQ07	10/15	CW07	10/18
9	CQ08	10/22	CW08	10/25
10	CQ09	10/29	CW09	11/01
11	CQ10	11/05	CW10	11/08
12	CQ11	11/12	CW11	11/15
13	CQ12	11/19	CW12	11/22
14				
15	CQ13	12/03		

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

Meeting Schedule

(tentative; see Canvas website course stream)

Week	Date	Lec	Topic	Notes Section
			—- Part 1 —-	
1	08/26	01	Introduction; Microscopic and Macroscopic Properties	0 - 1.6
	08/28	02	Temperature and Energy; Collision Frequency	1.7 - 2.2
2			no class	-
	09/04	03	Real Gases; Thermodynamic Definitions and Nomenclature	2.3 - 3.1
3	09/09	04	Thermodynamic Law and its Postulates; Expansion Work	3.2 - 4.1
	09/11	05	Heat, Work, Energy, Changes in State, and Reversibility	4.2 - 4.5
4	09/16	06	Enthalpy, Free Energy, and Reversibility	4.6 - 5.4
	09/18	07	Thermodynamic EOS; Adiabatic Work; Thermochemistry	5.3 - 5.B
5	09/23	08	Spontaneity; Combined Law Relations	6.1 - 6.A
	09/25	09	Thermodynamic Limits to Heat-Work Conversion	7.1 - 7.A
			—- Part 2 —-	
6	09/30	10	Mixing; Advancement; The Equilibrium Constant	8.1 - 8.8
	10/02	11	Solution Equilibrium; Single Component Phase Diagram	8.A - 9.1
7	10/07	12	Phase Equilibria; Surfaces and Interfaces	9.2 - 10.6
	10/09	13	Colligative Properties	11.1 - 11.6
8	10/14	14	Electrolytes	12.1 - 12.8
	10/16	15	Electrochemistry	13.1 - 13.A
			—- Part 3 —-	
9	10/21	16	Simple Chemical Kinetics	14.1 - 14.2
	10/23	17	Complex Kinetic Mechanisms	14.3 - 14.5
10	10/28	18	Transport Processes	15.1 - 15.5
	10/30	19	Electrolyte Conductivity	16.1 - 16.A
			—- Part 4 —-	
11	11/04	20	Statistics, Probability and Thermodynamics	17.1 - 17.4
	11/06	21	The Boltzmann Distribution; The Partition Function	17.4 - 18.1
12			no class	-
	11/13	22	Calculating Thermodynamic Properties	18.1 - 18.3
13	11/18	23	Units and Allosterism	18.A - 18.B
	11/20	24	Molecular Dynamics	19.1 - 19.3
14			no class	-
			no class	-
15	12/02	25	Review and Summary	0.0 - 19.D
	12/04	26	no class	

Course Resources and Ancillary Materials

Content

Textbook

This course covers material that is part of the core of any Physical Chemistry curriculum. Therefore, it is covered in many ways in many published, professionally edited and proofread textbooks. New Physical Chemistry textbooks are expensive, but recent but not current, editions can be acquired for little money and remarkable value. Get some. Use the Marston Library, https://marston.uflib.ufl.edu/ to peruse a large variety of text resources related to our course.

Course Notes

Notes guiding course topics and discussion are posted on the course website. The expectation is that these notes and lecture schedule will inform your preparation for our class meetings. It is not expected that these notes will be sufficient on their own for all learners to master the subject matter, as this is impossible.

As a draft document, the notes will be revised *constantly* through the term; Always refer to the *latest revision date* when reading or studying. The revision date is always contained on the first page of the document.

Our Jupyter/Python Server: https://jupyter2.chem.ufl.edu

This course will take advantage of modern computational tools to expedite mathematical derivations, process experimental data, and render hypotheses graphically. The platform most often used by professionals to easily and effectively interface with the widest variety of these tools is the Python programming language executed in a Jupyter notebook. Such an environment can be implemented on any device from a cell phone to a supercomputer cluster, and is done so routinely.

In order to aid in the mastery of such an environment, a course JupyterHub server has been set up for students in this course. It can be accessed with a web browser through the private URL https://jupyter2.chem.ufl.edu. This platform does not require any installation on your personal device although someday you will want to do that. Things to note:

- The servers address is only accessible on the UF campus network. If you are off campus or otherwise not connected to the campus network, a VPN tunnel must be initiated prior to connection. This is similar to the library database and other services protected by the UFIT firewall. If you are not familiar with the use of VPN, see https://it.ufl.edu/ict/documentation/network-infrastructure/vpn/.
- If you are registered for this course, an account has been created for you using your Gatorlink Username (GLID) as a login. (Your GLID is the name before the '@' symbol in your '@ufl.edu' email address) However, the password for the course server is NOT your gatorlink password. Your password will be set upon your first login.
  - Do not use the same password as your gatorlink credentials.
  - Do remember your password. If you forget your password, the reset process may cause a loss of your work.
- Use of our class server will expedite the instructor's ability to assist student mastery of the tools needed to make Physical Chemistry fun and easy. If you with to use your own Python instance, you still may need to upload your work to the class server for evaluation.

Grades

Course Grade Computation

Research has shown that assessing grades through a few, high-stakes, proctored activities (aka 'Exams') is not the best way to foster deep learning or long-term retention of concepts. Therefore, this course will attempt to have no mid-term or final exams. Course grades will be computed from the weighted-average of the earned percentages of each graded items described in section Course Activities, submitted by the individual student. The weighting factors of the activity categories are as follows:

Default Category Weights

Grade Category	weight %
Class Participation (CP)	25
Concept Quiz (CQ)	25
CourseWork (CW)	50

Alternate Category Weights

Grade Category	weight %
Class Participation (CP)	25
Concept Quiz (CQ)	12.5
CourseWork (CW)	12.5
Final Exam	**50**

If either the instructor or the student body indicate their dissatisfaction in the accuracy of the default grading method, or there is any indication of improper or dishonest behavior in the execution of the assignments, an alternate, more draconian, grading procedure will be activated. This scheme emphasizes a proctored, cumulative, extremely high-stakes Final Exam. This Final Exam, if necessary, is scheduled as per the Office of the Registrar for this section. If it is to occur, the activation of the alternate grading scheme for the course will be announced at least two weeks before the scheduled date of the final exam.

The grading scheme will generate an 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/UGRD/academic-regulations/grades-grading-policies/

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 (https://sccr.dso.ufl.edu/sccr/process/student-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: August 12, 2024—