



CHM4412:

Quantum Mechanics and Spectroscopy

Fall 2018 4 credit hours

Class Number (section) 11864

T R Periods 7-8 (13:55 - 15:50) JHH221

No (specifically) Required Textbook:

Useful texts include *the one you have* or something like:

Physical Chemistry, P. W. Atkins,

or similar titles by McQuarrie & Simon, Levine, Raff, Castellan

Every attempt will be made to provide complete course materials on our website, but you should have a physical [*sic*] textbook anyway...

See Brucat if you have questions...

Instructor: PJ Brucat

- Office location: CLB311
- Scheduled (group) office hours:
Monday's period 6, Wednesday's period 8,
and Friday's period 4
- Private office hours:
by Appointment, offer three choices (see below)
- Contact method: *Canvas Messaging only*

Course Website:

<https://ufl.instructure.com/courses/353739/>

All course materials, course communications, and many assessments will be delivered from within UF's eLearning system (Canvas) at the URL above. Please become familiar with our course website as soon as possible. Note that some of the materials there will be subject to change, so pay attention to all announcements. It is suggested that printing or static downloads of the content be avoided.

Course Goals: Successful completion of this course will enable the learner to

- Diagnose and exploit the underlying Quantum Mechanical principles in the analysis of Chemical systems and transformations
- Utilize a new perspective on the material Universe appreciating the concepts of coherence, quantum probability, the act of measurement, entanglement, mass, diffusion, and many other Quantum phenomena
- Profit from a broader and more precise methodology for asking questions about our physical world
- Taste the flavor of The Quantum World
- Become a better Scientist

		FALL SEMESTER 2018						
		S	M	T	W	T	F	S
Aug.	12	13	14	15	16	17	18	
	19	20	21	22	23	24	25	
	26	27	28	29	30	31		
Sept.								1
	2	3	4	5	6	7	8	
	9	10	11	12	13	14	15	
	16	17	18	19	20	21	22	
	23	24	25	26	27	28	29	
Oct.	30							
		1	2	3	4	5	6	
	7	8	9	10	11	12	13	
	14	15	16	17	18	19	20	
	21	22	23	24	25	26	27	
Nov.	28	29	30	31				
					1	2	3	
	4	5	6	7	8	9	10	
	11	12	13	14	15	16	17	
	18	19	20	21	22	23	24	
Dec.	25	26	27	28	29	30		
								1
	2	3	4	5	6	7	8	
	9	10	11	12	13	14	15	
	16	17	18	19	20	21	22	
	23	24	25	26	27	28	29	
	30	31						

Course Objectives: Mastery of the course material will be assessed in the following areas

- Knowledge
 - Postulates and formalism of Quantum Mechanics
 - Properties of simple QM systems (PiB, SHO, Hydrogen Atom, Hydrogen Molecule, *etc.*)
 - Features of common spectroscopic methods (UV-Vis, IR/Raman, $\mu\lambda$, NMR, *etc.*)
 - Classification of molecular symmetry
 - Properties of models applied to the description of Chemical Bonding
- Skills
 - Create a Hamiltonian operator for a given Chemical system
 - Apply Differential Equation methods to the solution of QM Problems
 - Identify and apply appropriate approximate methods to QM Problems
 - Apply methods of Linear Algebra to the solution of Quantum Chemical problems
 - Apply Group Theory to Quantum Chemical systems
 - Analyze and interpret Molecular Spectra

Course Operation and Philosophy The structure of the course consists of physical meetings twice a week in a classroom. Some of this time will be used in the traditional lecture method of teaching, some group discussion, and some learners working problems on the board with the remainder of the class helping. Research has shown that lectures are most effective when they are prepared for and reviewed. Therefore we will formalize this process with defined preparation and review activities, defined below.

Mediasite: All lectures in JHH221 will be recorded and posted in a [Mediasite Catalog](#)

Communication with your Instructor All course communications with your Instructor(s) are to occur within the Canvas environment using the embedded Announcement, Discussion, or Messaging tools (all grade-related discussion should exclusively use Canvas Messaging directly to the Instructor). Your Canvas account profile must be configured for immediate automatic notification of course announcements and course communications via the individuals preferred communication/email method. Do this now. Responsibility for receiving and responding to electronic course communication in a timely fashion is entirely that of the student.

Office Hours and Scheduled Meetings Office hours held by Brucat are intended for one-on-one discussion of a students standing in the class (grades), learning strategy and habits, remediation of specific hindrances to individual learning, and any other things not appropriate for group discussion. Private discussions will be held at times you arrange, since scheduled Office Hours are open to the class. If you want a meeting of this sort, message your instructor (from within Canvas, only) 3 options for meeting times that are convenient for you, and your instructor will reply with a choice that works best and a location for the meeting. Make sure to put at least three distinct time options in your initial message .

Attendance Your prompt attendance at all our scheduled class times is required. If you are unable to make a class for some reason, please message the Instructor (within Canvas) before the scheduled class time. Excused absences are defined by [University attendance policy](#). Unexcused absences will result in grade penalties at the discretion of the Instructor.

Etiquette Your polite, courteous, and civilized behavior is expected in all aspects of our course. This holds especially true for electronic and interpersonal communication with your peers and your Instructor.

Regrade Requests You have the right to ask for any assignment to be regraded if you suspect an error. Regrade requests must be received by the Instructor within 72 hours of the grade posting. Regrades will be performed only on the entire assignment. Since the process of regrading is to correct errors and make all grading consistent and fair, the grade may either increase or decrease as a result. Regrade requests must be submitted through Canvas.

Course Activity Types

Discussion Preparation Before every class meeting, a preparation assignment will be posted. At the very least it will include some reading, and also a look at relevant problems (CourseWork or CW, see below) that will be submitted after the lecture is given. Lecture preparation Assignments are not graded.

Lecture Review After each lecture, there will be a Community Review assignment delivered in [VoiceThread](#). The assignment will typically be to post comments on the lecture notes displayed, but other activities may be requested. Read the assignment instructions for details.

CourseWork (CW) Traditional classes have you, the student, work exemplary problems to cement your mastery. These are often worked outside of class, usually alone. We are going to work those problems in class, together. A portion of your grade will be derived from these problem sessions, so be prepared.

Quizzes Periodically throughout the term, short on-line assessments will be delivered through the course website.

Exams There will be four in-class exams during the term. These are typically 5-6 page white-space closed-book tests, with a page or two of given information (fact sheet) to assist your work. These Exams will be graded and reviewed in class by your instructor.

All activity dates and grades are posted in Canvas

Course Grade Computation: Course grades will be computed from the weighted-average of the earned percentages of each graded item submitted by the student. The weighting factors are as follows:

Category Weights		Grade Percentages									
Grade Category	weight %	Grade	A	A-	B+	B	B-	C+	C	D	E
Preparation	0	Minimum percentage	87.5	80.0	77.5	72.5	70.0	67.5	60.0	50.0	< 50.0
Lec Review	10										
Quizzes	10										
CourseWork	10										
Exams	70										

UF's Grading Policy: <http://www.registrar.ufl.edu/grades/grade政策.html>

Honesty and Truthfulness: Students, faculty, and all participants in UF's Academic activities are bound by the [Honor Code](#). Moreover, ethical, moral, and professional behavior is expected and required of all participants in this course.

Accommodations: Students with disabilities may request special accommodations through the Dean of Students. <https://drc.dso.ufl.edu/>

Counseling: Useful non-academic services are available in many forms at UF. A good source of information is the Counseling and Wellness Center: <http://www.counseling.ufl.edu/cwc/>

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

— PJ Brucat 07/23/2018 —