NEW YORK UNIVERSITY

Quantum Mechanics and Spectroscopy

Department of Chemistry

CHEM-UA-651

Spring semester, 2017

22 January 2017

CHEM UA 651 Syllabus: General Information

Instructor:

Prof. Daniel B. Turner Office: Silver 704 Phone: 212–992–6541 Email: dturner@nyu.edu

Lectures:

Tuesdays & Thursdays, 2:00 PM – 3:15 PM, Meyer 102

Recitations:

You must register for one of the recitation sections for this course. The instructor is Prof. Dubravko Sabo, dubravko.sabo@nyu.edu.

Sec 101: Mondays, 8 AM – 9:15 PM, 25 W 4th Street, Room C-13

Sec 102: Mondays, 11:00 AM – 12:15 PM, Silver 508

Sec 103: Mondays, 12:30 PM – 1:45 PM, Silver 407

Office hours:

Tuesdays, 10:45 PM – 12:00 PM, or by appointment in Silver 704

Recommended Text:

Physical Chemistry: A Molecular Prospective by McQuarrie and Simon

Additional course materials will be posted on the NYU Classes page.

It is important that you read the textbook!

Alternate Texts:

Introduction to Quantum Mechanics by Griffiths

Symmetry and Spectroscopy by Harris and Bertolucci

Physical Chemistry by Laidler, Meiser, and Sanctuary

Physical Chemistry by Atkins and de Paula

Recommended Software:

The use of software is strongly encouraged especially for plotting. Options include: Matlab, Mathematica, Julia, Origin, Python, Octave, Scilab, and LoggerPro. I do not recommend Excel. Octave, Python, Julia (*http://julialang.org/*), and Scilab are freely available. Matlab and Mathematica are available for free to NYU students via the VCL:

1. log in into home.nyu.edu, click "VCL Login" button at the bottom left corner, there will be a new page generated.
2. click "Log In to the VCL NOW!", you will see *** Files saved to the VCL will be deleted when quitting an application. To ensure that you retain your files, save them to your local hard drive. ***

3. enter your NetID and password, LOG IN.
4. find Mathematica and click it, you will be asked to install a plug-in. Install it and click Mathematica again, you will go into Mathematica.
5. after your file is done, save it to your local hard drive! To run the file on vcl Mathematica, choose add to path so that it can be found.

Prerequisites:

1. Math-UA 0122 *and*
2. Phys-UA 0012 or Phys-UA 0093 *and*
3. Chem-UA 0102 or Chem-UA 0104 or Chem-UA 0110 or Chem-UA 0112 or Chem-UA 0126 or (Scien-AD 107 *and* Scien-AD 108 *and* Scien-AD 110)
4. with a minimum grade of C.

In other words: Two semesters of general chemistry, two semesters of university introductory physics (with calculus), and at least two semesters of university calculus.

Course Site:
The main course site is the NYU Classes page.

Tutoring:

1. The University Learning Center provides free peer tutoring:
   http://www.nyu.edu/students/undergraduates/academic-services/undergraduate-advisement/academic-resource-center/tutoring-and-learning.html

2. In addition, Phi Lambda Upsilon (PLU) will provide peer tutoring sessions. Dates, times, and locations will be announced on the course website. They will hold relevant mathematics reviews early in the semester and exam preparation sessions during the semester.

CHEM UA 651 Syllabus: Learning and Assessment

Problem sets:

Problem sets will be posted on the NYU Classes page. Problems sets are due at the beginning of the recitation session on the due date, and they will be *graded on completeness*.

Readings:

Some additional materials for deeper discussions will not be covered in full in class, but will be assigned as reading materials. The content will be part of the material assessed on the problem sets, exams, and quizzes.

Quizzes:

Quizzes will be given during recitation. Each quiz will be composed of 1 or 2 questions similar to recent problem-set questions. Only calculator allowed. Common equations and constants will be provided. The lowest quiz score will be dropped in final grade calculation.

Assessment opportunities:

Problem sets	10%
Quizzes	15%
Midterm exam 1	22.5%
Midterm exam 2	22.5%
Final exam	30%

You are welcome to work together on the problems sets, with the understanding that the final product reflects your understanding and is not copied from someone else.

Exams:

Only calculator allowed. Common equations and constants will be provided.

If you will miss a midterm examinations because of illness, you must contact Professor Turner by email *before the start of the exam* and provide a doctor's note explaining your absence. *No make-up midterm exams* will be given; the exam grade will be composed of the exams taken.

A make-up will be given for *the final exam only* under extraordinary circumstances that must be discussed with Professor Turner prior to the exam. In the singular cases where approval is granted, a grade of incomplete will be given for the course and the make-up will be scheduled for the Fall 2017 semester.

CHEM UA 651 Syllabus: Learning and Assessment

Working problems is the heart and soul of learning quantum mechanics, and physical chemistry in general. The only way that you can be sure that you understand a concept is to solve problems associated with it. This takes time and effort. There are things that you can do to help yourself:

1. Sadly, nobody cares if you solve a problem on the problem set. They have all been solved before, so if you solve them you will not become famous or save the world. The only reason you work problems is to learn.
2. Budget your time so that you don't have to work on an overwhelming number of problems at a time. Try to do a few on the same day that you receive the problem set. Then work on the others consistently during the week. This will make the problem sets much more efficient at helping you learn.
3. You can do the problems. I don't assign problems that you cannot do.
4. First understand what the problem is asking you to do. There is a tendency to try to start solving the problem before fully understanding the question.
   (a) Read the question carefully.
   (b) Try to think about what topic(s) in lecture and in the notes relate to the problem.
   (c) Do not worry about not knowing how to solve it yet.
   (d) Just identify the general ideas that you think you might need.
   (e) Determine wether you need to approach the problem mathematically, conceptually, or both.
   (f) If the question is long, try to identify subsections of it.
5. For problems that require a mathematical approach
   (a) Do not be afraid. Try to figure out what mathematical techniques you need to express the solution to the problem.
   (b) Do the math; either you will be able to do this or you won't. It might take some review on your part.
   (c) Always check to see if the math makes sense when you are done.
6. For problems that require a conceptual approach
   (a) Make sure that the physical idea that you are using in your response is correct. If you are not sure, start with a related concept that you understand better.
   (b) Look for self-consistency. Does you final answer jive with what you know?

CHEM UA 651 Syllabus: Calendar

http://www.nyu.edu/registrar/calendars/university-academic-calendar.html
http://www.nyu.edu/registrar/registration/final-exam-schedules.html

Topic	Mon (**recitation**)	Tues (**lecture**)	Thurs (**lecture**)
fall of classical physics	*23 Jan*	24 Jan	26 Jan
(Ch 1)	*no recitation*	(PS0 & PS1 out)	
Schrödinger Eqn & PIB	30 Jan	31 Jan	2 Feb
(Ch 2, 3)			(PS2 out)
postulates of QM	6 Feb	7 Feb	9 Feb
(Ch 4)	PS1 due		(PS3 out)
harmonic oscillator	13 Feb	14 Feb	16 Feb
(Ch 5)	PS2 due		(PS4 out)
midterm 1	*20 Feb*	21 Feb	23 Feb
	Presidents' Day	PS3 due (PS5 out)	**Exam 1**
rigid rotor & H atom	27 Feb	28 Feb	2 Mar
(Ch 5, 6)	PS4 due		(PS6 out)
continue hydrogen atom	6 Mar	7 Mar	9 Mar
(Ch 6)	PS5 due		(PS7 out)
no class, spring recess	*13 Mar*	*14 Mar*	*16 Mar*
approximation methods	20 Mar	21 Mar	23 Mar
(Ch 7)	PS6 due		(PS8 out)
multiple-electron atoms	27 Mar	28 Mar	30 Mar
(Ch 8)	PS7 due		(PS9 out)
midterm 2	3 Apr	4 Apr	6 Apr
			Exam 2
chemical bond: diatomics	10 Apr	11 Apr	13 Apr
(Ch 9)	PS8 due		(PS10 out)
polyatomics, comp chem	17 Apr	18 Apr	20 Apr
(Ch 10, 11)	PS9 due		
spectroscopy and lasers	24 Apr	25 Apr	27 Apr
(Ch 13–15)	PS10 due		
statistical thermo intro	1 May	2 May	4 May
(Ch 17, 18)			
recitation only	8 May	*9 May*	*11 May*
final exam	*15 May*	16 May	
		Final (2–3:50 PM)	