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Syllabus (Fall 2019)
Chemistry 562: Physical Chemistry II

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> The policies and regulations contained in this syllabus are subject to change at any point. Such changes will be announced in class and/or posted on the course website. The syllabus has been compiled to be as complete as possible but is by no means a binding document.

General Info

Instructor:	Prof. **Jörg C. Woehl**
Office:	Chemistry Building (CHM), Room 343
Office hours:	Open door
Email:	woehl@uwm.edu
Phone:	414-229-5223

Class Meeting Times:	Monday, Wednesday, and Friday, 9:00-9:50 am
Class Location:	CHM 197
Discussion Group:	Friday, 1:00-1:50 pm in CHM 193
Teaching Assistant:	Quintus Owen (qowen@uwm.edu)
TA Office hours:	Wednesday, 1:00-2:00 pm in CHM 218
First Day of Class:	Wednesday, September 4
Last Day of Class:	Wednesday, December 11
Midterm 1 (in-class):	Monday, October 14, 9:00-9:50 am
Midterm 2 (take-home):	Monday, November 11; due following Monday at 9:00 am
Final Exam:	Monday, December 16, 10:00-12:00 noon (CHM 197)

Course Objectives

This lecture course covers quantum mechanics (as it applies to the chemical sciences), chemical kinetics, and statistical mechanics (thermodynamics). In contrast to "Physical Chemistry I" (Chem-561), the approach we take in this course is purely microscopic. Starting with electrons and nuclei, we will arrive at a quantum-mechanical description of the atom, and use the same approach to understand chemical bonding, reactions, and thermodynamic properties.

Individual Particles

Quantum mechanics is used to describe the motion of microscopic particles, and we will introduce the concepts using the historical evolution of quantum theory. The ideas will be tested by looking at the radiation (light) emitted by atoms and molecules (spectroscopy), focusing on vibrational and rotational motion. The energies of electrons and the spectroscopy of the hydrogen atom will be discussed, followed by an examination of atoms with several electrons and the effect of magnetic fields on the energies of the atoms (Zeeman effect).

Chemical Bonding
The ideas of quantum mechanics will be extended to chemical bonding. Simple models that explain the formation of chemical bonds will be discussed.

Treatment of Collections of Molecules
Since chemical reactions are generally carried out with large numbers of atoms or molecules ($\sim 10^{23}$) we will use a statistical approach to examine their properties. This will include a discussion of probability distributions (Boltzmann distribution function). We will use these ideas to calculate thermodynamic functions (internal energy, entropy) and introduce the idea of the Partition Function (Z). This will be calculated for a number of systems and we will discuss the ways in which this is applied, in particular, to the calculation of equilibrium constants and its application to chemistry.

Required Textbook
David W. Ball: "Physical Chemistry" (2nd ed.), Cengage, 2014. Chapters 9-20. ISBN 9781133958437.
Available through UWM's Virtual Bookstore uwm.ecampus.com.
Recommended, but optional:
"Student Solutions Manual" (2nd ed.), Cengage, 2014. ISBN 9781285074788. UWM Libraries Call Number QD453.3 .B352x 2015 (on course reserve).
Available through UWM's Virtual Bookstore uwm.ecampus.com.
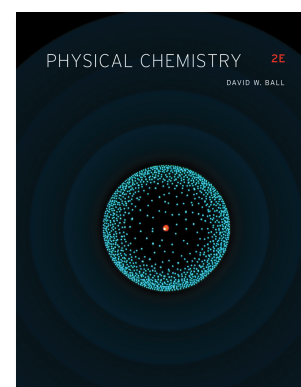
Supplemental Textbooks
- Donald A. McQuarrie and John D. Simon: "Physical Chemistry: A Molecular Approach", University Science Books, 1997. UWM Libraries Call Number QD453.2 .M394 1997 (on course reserve)
- Peter Atkins and Julio de Paula: "Physical Chemistry" (9th ed.), W. H. Freeman and Company, 2010. UWM Libraries Call Number QD453.2 .A88 1998 (6th ed.).
- Robert J. Silbey, Robert A. Alberty, and Moungi G. Bawendi: "Physical Chemistry" (4th ed.), John Wiley & Sons, 2005.
- Horia Metiu: "Quantum Mechanics", Taylor & Francis, 2006.
- Horia Metiu: "Statistical Mechanics", Taylor & Francis, 2006.
- Horia Metiu: "Kinetics", Taylor & Francis, 2006.
- Donald A. McQuarrie: "Mathematical Methods for Scientists and Engineers", University Science Books, 2003. UWM Libraries Call Number QA37.3 .M36 2003 (on course reserve).

Course Prerequisites
"Chemistry 562: Physical Chemistry II" (Chem-562) requires junior standing and a grade of **C or better** in Chem-561 ("Physical Chemistry I"). If you do not have the proper prerequisites, you need to obtain my consent to take this course.
The prerequisite course Chem-561 may **not** be taken for credit subsequent to the earning of credit in Chem-562!
In order for you to be successful in this course you will need to be at ease with (elementary and linear) algebra, differential and integral calculus. If you are not

sufficiently familiar with these topics, you should consider taking Chem-562 at a later time, once you have acquired these skills.

Lectures
You are expected to attend all lectures and discussion groups. There is generally a strong correlation between students who receive good grades and those who attend class and discussion groups on a regular basis. Please contact me (preferably by email) if you are unable to attend a class or discussion group.

Before attending a lecture, you should prepare the material by reading the corresponding textbook sections so that you can follow the presentation more easily and ask questions about topics that you have not (or not fully) understood. Also, work through the example problems scattered throughout the text; then, try to solve them on your own. Working problems is the best way to learn and check your comprehension of the material. We will work on problem solving during the discussion sections. I will sometimes suggest a number of simpler practice problems on the course website.

Course Website
Canvas: uwm.edu/canvas/. For information on how to use Canvas, please visit uwm.edu/canvas/students/.
Course material will be made available on Canvas. It is expected that you visit the course website regularly as important information and announcements may be posted there as well.

Problem Sets
Problems illustrating the use and application of the theory will be discussed during discussion sections. Homework problems will be assigned on a weekly basis and collected during class one week later. Some problems will be graded and returned (typically one week later) and discussed during discussion section. You may work on homework problem sets either on your own or in groups with other students; I highly recommend working in groups as it allows you to discuss the topics with others and to formulate strategies for problem solving, thus reinforcing your understanding of the material.

Grading
The course will be graded based on problem sets and examinations as follows:

Homework Problems	20%
Midterm 1 (in-class)	25%
Midterm 2 (take-home)	25%
Final Exam (in-class)	30%
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Total	100%

Midterm 1 is an in-class exam and will be held during regular lecture time. Only a calculator (programmable or non-programmable) and a single sheet of paper with handwritten notes (recto-verso) are allowed. No books or other material are admitted.

If you know that you will miss Midterm 1, please contact me as soon as possible (preferably by email). If you are missing Midterm 1 for a valid and justifiable reason, I will make arrangements so that you can take a make-up exam within one week after the scheduled date. If you miss Midterm 1 without justified excuse, you are not eligible for taking a make-up exam.

Midterm 2 is a take-home exam and will be handed out and posted to Canvas after the lecture. The midterm will cover all topics discussed in class and problem sets in a format similar to the problem sets. No class will be held on Wednesday during midterm week. No time extensions or make-up exam will be given for the take-home midterm. If you are unable to turn it in during class, you may upload it to the Canvas dropbox.

The *Final Exam* is comprehensive. Again, only a calculator (programmable or non-programmable) and a single sheet of paper with handwritten notes (recto-verso) are allowed. No books or other material are admitted.
If you are unable to take or complete the final exam due to illness or other unusual and substantiated cause beyond your control, an incomplete ("I") will be given *if you can provide proof for such cause*. According to UWM policy, a course marked incomplete must be completed (in this case by taking a make-up final exam) during the next succeeding semester, excluding summer sessions and UWinterim; otherwise, the grade of "I" will lapse to "F".

Tentative Schedule

	Week	Topic
1	Sep 4 - Sep 8	Historic Experiments leading to Development of Quantum Mechanics
2	Sep 9 - Sep 15	Schrödinger Equation
3	Sep 16 - Sep 22	Applications of Schrödinger Equation: Particle-in-a-box Harmonic Oscillator
4	Sep 23 - Sep 29	Applications of Schrödinger Equation: Harmonic Oscillator Rigid Rotor
	Sep 30	Last day to drop full-term courses without "W" on record
5	Sep 30 - Oct 6	Formalism of Quantum Mechanics
6	Oct 7 - Oct 13	Applications of Schrödinger Equation: Hydrogen Atom

Week		Topic
7	Oct 14 - Oct 20	**Midterm 1 (in-class), Monday, Oct 14** Introduction of Spin Many-Electron Atoms
8	Oct 21 - Oct 27	Spectroscopy of Atoms
9	Oct 28 - Nov 3	Molecules and Bonding
10	Nov 4 - Nov 10	Molecules and Bonding
	Nov 10	Last day to drop or withdraw from full-term courses
11	Nov 11 - Nov 17	**Midterm 2 (take-home), Monday Nov 11 - no class on Wednesday, Nov 13** Rotational and Vibrational Spectroscopy
12	Nov 18 - Nov 24	Rotational and Vibrational Spectroscopy
13	Nov 25 - Nov 26	Statistical Thermodynamics - Basics
	Nov 27 - Dec 1	Thanksgiving Recess
14	Dec 2 - Dec 8	Applications of Statistical Thermodynamics
15	Dec 9 - Dec 12	Applications of Statistical Thermodynamics
	Dec 16	**Final Exam 10:00 am - 12:00 noon (CHM 197)**

Workload
Besides attending lectures and discussion groups, you should expect to take at least 50 hours over the course of the semester reading the textbook and lecture notes and solving homework and example problems to double-check your comprehension of the material.
Weekly homework problem sets and practice problems will be given, which will take you *at least* 5 hours each although the exact amount of time will vary by student and by week and will depend largely on your mathematical background.
You should reserve at least 10 hours to study for and take the final exam.
All told, this class is likely to take about 150 hours of your time.
This workload is only an estimate and will vary from student to student. Also, it should be understood that you are assessed on your performance, not on the time put into the course.

Policies

If you will need accommodations in order to meet any of the requirements of this course, please contact me and the UWM Accessibility Resource Center (ARC) as soon as possible. Special accommodations for students with disabilities can be provided, but their timely implementation can only be insured if the ARC is contacted ahead of time. For details see uwm.edu/arc/getting-started/.

Department of Chemistry and Biochemistry policies are posted on bulletin boards in the department.

UWM policies related to students with disabilities, religious observances, students called to active military duty, incompletes, discriminatory conduct, academic misconduct, complaint procedures, grade appeal procedures, and final examination requirements can be consulted at uwm.edu/secu/syllabus-links/.

Academic Misconduct

Cheating on an exam or other graded material will automatically result in a grade of zero (as a minimum consequence); failure in the course and referral to the Dean may also occur. Academic dishonesty in any form will not be tolerated.

"Academic misconduct is an act in which a student seeks to claim credit for the work or efforts of another without authorization or citation, uses unauthorized materials or fabricated data in any academic exercise, forges or falsifies academic documents or records, intentionally impedes or damages the academic work of others, engages in conduct aimed at making false representation of a student's academic performance, or assists other students in any of these acts."

"Prohibited conduct includes cheating on an examination; collaborating with others in work to be presented, contrary to the stated rules of the course; submitting a paper or assignment as one's own work when a part or all of the paper or assignment is the work of another; submitting a paper or assignment that contains ideas or research of others without appropriately identifying the sources of those ideas; stealing examinations or course materials; submitting, if contrary to the rules of a course, work previously presented in another course; tampering with the laboratory experiment or computer program of another student; knowingly and intentionally assisting another student in any of the above, including assistance in an arrangement whereby any work, classroom performance, examination or other activity is submitted or performed by a person other than the student under whose name the work is submitted or performed."

(From: Office of the Provost and Vice Chancellor)