CHEMISTRY 301: ELEMENTS OF PHYSICAL CHEMISTRY
Course Syllabus and Schedule – Fall 2020
Revised 8/15/20

Time and "Location": 8:30 – 9:20 AM MWF
ZOOM ROOM: 963 8770 3716
https://duke.zoom.us/j/96387703716

Instructor: Kevin Welsher

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Office hours: TBD by Doodle Poll
or by e-mail appointment

Textbook: *Required*: "Physical Chemistry for the Chemical Sciences," by Raymond Chang and John W. Thoman, Jr. (University Science Books, 2014).
Electronic copy also available through Duke Library.
Link: https://find.library.duke.edu/catalog/DUKE007496608

Optional: "Problems and Solutions to accompany for Physical Chemistry for the Chemical Sciences by Chang and Thoman," Helen Leung and Mark Marshall (University Science Books, 2015).

Lecture Notes/Course Reader: Available on Sakai

Course Overview: This course will survey several main topics of modern physical chemistry, including quantum chemistry, molecular structure, and molecular spectroscopy, which describe *microscopic* properties of systems; thermodynamics and chemical kinetics, which describe *macroscopic* properties of systems; and statistical mechanics, which provides the *connection* between microscopic and macroscopic properties. Because the course attempts to treat all these topics in a single semester rather than in the more traditional two-semester format, there will necessarily be compromises in breadth and depth. The goal will be to provide a firm grounding in the essential principles of physical chemistry that can be used as a foundation for other chemistry and science courses, and for more advanced topics or applications of physical chemistry that might be encountered. This course will also provide the theoretical background for the experiments in the associated laboratory course, CHEM 301L, offered in the spring semester. The course will cover selected material from Chapters 10-14, 17, 1, 3-5, 8, 15 and 20 of the text. There is no ideal text for this course, and students are encouraged to consult the instructor for suggestions for further reading. The attached schedule is intended as an approximate, general outline; the order of topics will be as indicated, but the exact dates and amount of time devoted to each topic may change as the semester progresses. The exam dates are fixed, however.

Course Structure and Resources: The course will be taught synchronously online via Zoom. Lectures will be held 8:30-9:20 AM MWF in the Zoom room listed at the top of this document. Lecture attendance is not required, but is recommended to keep up with the fast pace of the course.

All lectures will be recorded and available on demand. There are several online resources that will be used to supplement the lectures:

- **Sakai** – Home for general course information where I will post lecture notes for each lecture as well as homework assignments.
    - **Link:** https://sakai.duke.edu/x/yzArYr
- **Lecture Notes / Class Reader** – A pdf document will be available on Sakai that includes lecture notes for the entire semester. We will not follow the book in order, so this is the best way to follow along with the class.
- **Piazza** – There will be a Piazza site for the course. This is great place to work through tough topics. No better way to be sure you know something than to answer someone else's questions!!
    - **Link:** piazza.com/duke/fall2020/chem301002f20
- **Warpwire** – There will be a Warpwire site to host videos to supplement lecture material. Videos are short and meant to review tricky concepts. More info on the supplemental videos will be given at the start of the course.
    - **Link:** https://warpwire.duke.edu/w/LREEAA/

Exams and Course Grade: There will be three midterm exams and each will contribute 16% to the course grade. The final exam will be cumulative and will contribute 32% to the course grade. The final portion of the grade (20%) will be from the additional homework problems mentioned below. Letter grades will be assigned according to the distribution of total scores. Midterm and final exams will be administered via Gradescope. They will be composed of a timed multiple choice/short answer section and a set of longer problems which will function as a take-home exam. Prior to the first midterm I will post a practice exam on Gradescope so that everyone is comfortable with the format.

Homework Problems: One of the main ways you learn physical chemistry is through application, e.g. by working problems. I will assign problems for you to work on an approximately biweekly basis. Some will be from the text; these will not be collected or graded, and you can use the answers in the back of the text or Solutions Manual to check your work. Try as many of the other problems for each Chapter as you have time for. Do not look at the solutions manual until you have first attempted the problems yourself or you will not learn from them. Even if you are unable to solve a problem, you will learn more and the answer will mean more if you first spend time "messing around" trying to find the solution. You may wish to form (virtual) study groups to work on the problems and discuss the material. I will also assign a few additional problems in each problem set for you to work out and turn in; you should attempt to do these on your own and you should write up your solutions on your own (if you receive any help from another student, the nature and extent of that help should be noted on your work). These extra problems will be graded on a "course-grained" scale; 2 = good, substantially correct solution; 1 = good effort; 0 = insufficient effort. Also, some of the exam problems may be closely related to the homework problems.

Academic Dishonesty and Cheating
All students are expected to abide by the Duke Community Standard. Any and all cases of academic dishonesty will be referred to the Office of Student Conduct. If you are found guilty of

cheating or other academic dishonesty, in addition to any action that the Conduct Board takes, and in addition to receiving a zero grade on the assignment in question, you may receive an F in the course. For additional information see: http://www.integrity.duke.edu and http://www.studentaffairs.duke.edu/conduct.

Approximate Lecture Schedule and (Fixed) Exam Dates:

Date	**Topic**	**Related Sections in Chang and Thoman**
17-Aug	Lecture 1: Particles and Quantization of Energy	10.1-10.3
19-Aug	Lecture 2: de Broglie, the Schrodinger Equation, and Wavefunctions	10.4-10.8
21-Aug	Lecture 3: Operators, Heisenberg, and Soluble Models of the Schrodinger Equation	10.6-10.8
24-Aug	Lecture 4: Particle in a box	10.8-10.10, 10.12
26-Aug	Lecture 5: Harmonic Oscillator	11.3
28-Aug	Lecture 6: Rigid Rotor and the H Atom	10.11, 11.2
31-Aug	Lecture 7: H Atom (cont.)	12.1-12.5
2-Sep	Lecture 8: Electron Spin, Extension to Multi-electron Atoms, Approx Methods	12.6-12.10
4-Sep	Lecture 9: Chemical Bonding and LCAO-MO	13.1-13.4
7-Sep	Lecture 10: LCAO-MO multi-e	13.2-13.4
9-Sep	Lecture 11: Hybrid Orbitals, Huckel Theory	13.6-13.7
11-Sep	Lecture 12: Intermolecular Forces	17
14-Sep	**MID-TERM EXAM #1 (Lectures 1-10)**	
16-Sep	Lecture 13: Intro to spectroscopy, absorption and emission, transition dipoles	14.1
18-Sep	Lecture 14: Rotational and Vibrational Spectra	11.2-11.3
21-Sep	Lecture 15: Rovibrational and Vibronic Spectra	11.2-11.3, 14.1
23-Sep	Lecture 16: Emission from Excited States	14.2
25-Sep	Lecture 17: NMR Part 1 - Shielding, Lenz's Law, and Chemical Shifts	14.6
28-Sep	Lecture 18: NMR Part 2 - Spin-spin Coupling, Magnetic Anisotropy, Rate Processes	14.6
30-Sep	Lecture 19: NMR Part 3 - FT-NMR	14.6

2-Oct	Lecture 20: Intro to Thermo, Equation of State, State Functions, Reversible and Irreversible Paths	1
5-Oct	Lecture 21: Exact Differentials, Work, Heat, and the First Law of Thermodynamics	3.1, Appendix 3.1
7-Oct	**MID-TERM EXAM #2 (Lectures 11-19)**	
9-Oct	Lecture 22: Calorimetry, Enthalpy, Heat Capacities, Ideal Gas Expansion	3.2-3.4
12-Oct	Lecture 23: Application of 1st Law to Phase Changes, Chemical Rxns	3.5, 3.7
14-Oct	Lecture 24: Spontaneity, Entropy, and the Second Law	4.1-4.4
16-Oct	Lecture 25: Application of 2nd Law to Phase Changes, Heat Engines/Pumps, Combined 1st and 2nd Laws	4.2-4.5, 5.2
19-Oct	Lecture 26: Entropy of Mixing, the 3rd Law, Absolute Entropy	4.6, 5.1
21-Oct	Lecture 27: Free Energies (A,G), Spontaneity, and Equilibrium	5.1, Appendix 5.1
23-Oct	Lecture 28: Free Energies and Work, Application to Phase Changes and Chemical Rxns	5.3-5.6, 6.2
26-Oct	Lecture 29: Chemical Potential and Equilibrium	6.2, 6.3, 8.1
28-Oct	Lecture 30: Equilibria Cont., Phase Equilibria	8.1-8.5
30-Oct	Lecture 31: Rate Laws	15.1-15.2
2-Nov	Lecture 32: Reaction Mechanisms and the Steady-State Approximation	15.3-15.4
4-Nov	**MID-TERM EXAM #3 (Lectures 20-30)**	
6-Nov	Lecture 33: Lindemann Mechanism, Enzyme Kinetics, Temperature Dependence of the Rate Constant	15.3-15.5
9-Nov	Lecture 34: Boltzmann Equation and the Microscopic Picture of Entropy	4.2, 4.7, 4.8
11-Nov	Lecture 35: Canonical Ensemble and Partition Functions	20.1-20.4
13-Nov	Lecture 36: Distinguishable and Indistinguishable Particles and Two-level Systems	20.3

16-Nov	Lecture 37: Ideal Gases	20.4
(if time allows)	Lecture 38: Molecular Interpretation of Heat and Work	
22-Nov	**FINAL EXAM (Cumulative, Lectures 1-38, 9AM to 12PM)**	