Physical Chemistry uses the theoretical structures and tools of Physics to study and predict the physical, thermal, electrical, and chemical properties of the matter that makes up our world of experience, including all living matter. It is guided by a few central ideas that illuminate many physical and chemical properties of matter, and understanding these ideas will provide a basis from which you can approach a wide range of problems. Among these problems are key concerns in today’s world such as the magnitude of the energy demands of our society and the presence of toxins in our environment. This course is the first semester of a two-semester sequence that introduces the key ideas and methods of physical chemistry, and it will focus on macroscopic approaches (principally Thermodynamics and Chemical Kinetics). The second semester will examine microscopic approaches (Quantum Mechanics, Spectroscopy, and Statistical Mechanics).

My goals for you in this course are that you:
1) Understand physical chemistry’s central ideas;
2) Be able to articulate the strengths and limitations of idealized models in chemistry;
3) Value the beauty and scope of thermodynamics;
4) Know the general approaches people use to control chemical processes;
5) Be able to evaluate claims for alternative energy sources
6) Understand why no substance is ever completely pure and that trace levels of contaminants, including harmful ones, are inevitable.

Course Objectives. Your objectives in this course include that you learn:

1. The fundamental laws of thermodynamics and how to use these laws to analyze physical and chemical processes.
2. How to calculate if a process can occur spontaneously, how to calculate the maximum amount of useful work that can be extracted from the process, such as the chemical reaction in a fuel cell. If it cannot occur spontaneously, you be able too calculate is the minimum energy that must be applied for the change to occur.
3. Where to locate thermodynamic data of common chemical compounds and how to use this data.
4. Develop facility in the use thermodynamic data to solve for equilibrium concentrations as a function of Temperature and Pressure.
5. To be able to interpret phase diagrams for both pure substances and mixtures.
6. What is meant by an ideal gas and solution and why are real gases and solutions not ideal.
7. How to quantitatively treat non-ideal solutions and gases.
8. To analyze the reactions that take place in electrochemical cells, and how to compare different types of batteries.

9. The principle contributions to intermolecular potentials and how these effect thermodynamic properties of substances.

10. The theory of transport properties and how this is used to predict the rate of non-equilibrium processes, such as diffusion and thermal conductivity.

11. The methods to quantitatively treat the rates of chemical reactions.

12. The ways that chemists break down complex chemical processes in terms of elementary chemical reactions and use these to predict the kinetics of the overall reactions.

13. The Haber-Bosch process for production of ammonia, including how both thermodynamic and kinetic factors are controlled to maximize yield and minimize energy costs. Also, you will learn how this single chemical process is fundamental to our feeding at least half of the present human population.

14. Some of the important sets of coupled reactions that are important in atmospheric chemistry and human influence on the atmosphere.

15. To use the Mathcad program to solve analytical and numerical problems.

**Required Course Materials:**
Principle Text: *Physical Chemistry*, 4’th edition by Robert J. Silbey, Robert A. Alberty and Moungi G. Bawendi. A companion guide has worked out solutions for all the odd numbered problems from the back of each chapter and is likely worth you obtaining a copy. The book store has located a large number of used copies – I suggest you purchase one as a new edition of this text will be issued in 2013.

You will be required to use **Mathcad**. This program can be run through the web using UVa “Hive” and is also available at some of the campus computer clusters, but I suggest you purchase a copy from the book store, which is available for a modest price due to a UVa site license. One problem is that Mathcad only runs under Windows, not the Mac operating system. With the dramatic increase in Mac market share, I hope they will return to supporting that platform. At present, I run Mathcad using **Parallels Desktop**, which allows me to run Windows applications on my Mac OSX computer and find it works well. To install Parallels, you need to have a Windows Operating system, which also can be purchased from the bookstore at **modest cost**.

You must have an IClicker and register it with Collab. Version 1 of the IClicker is fine.

**Course Prerequisites:** I have designed this course assuming that you have a working knowledge of differential, integral, and multivariable calculus, material covered in UVa’s introductory chemistry courses, and introductory physics. If you are currently taking Introductory Physics, please see me and we can explore if taking this course at this time makes sense for you.

**Mathematics.** Physical Chemistry makes more extensive use of Mathematics than other areas of chemistry that undergraduates are likely encounter, particularly the use of calculus, including multivariable calculus. This is often intimidating to students but
cannot realistically be avoided without loss of much of the substance of the subject. A part of the power of Physical Chemistry is that it allows for quantitative predictions, both from first principles in simple cases (ab initio), and from empirical data (often seemingly unrelated to what one wants to calculate) in others. The mathematics appears in two distinct ways. One is the formal mathematical derivation of results. Thermodynamics, especially, abounds with such examples. You need to review calculus, especially if you have made only sporadic use of these tools in the last several years. The Mathematical background section in the appendix of the text is a good place to start.

The second area that students often find mathematically demanding is computation, both numerical and symbolic. The development of computational and symbolic computer packages has changed how scientists, including chemists, approach such problems. The use of such packages removes much of the drudgery and numerical errors from calculations and allows treatment of much more realistic problems, but it requires development of other skills to effectively use the programs. There are several popular packages, but in this course I will be using Mathcad. Mathcad documents (known as worksheets) look like a notebook page and allow natural mixing of equations and text. Mathcad does both symbolic and numerical calculations (though it is stronger for the later). It also does unit calculus and automatically converts units. Many unit are built in and others can be defined.

Reading assignments will be given before each class and you are expected to read the material before it is covered in class. The reading will include material from the textbook, sections of my “lecture notes,” Mathcad documents, and other material, including those that relate the course content to broader scientific and/or societal issues. Mathcad documents will largely be ones I have prepared to teach course content as well as demonstrate how different calculations can be done using this tool. I will not explicitly lecture on the material covered in the reading assignments! In class time will largely be used to 1. Answer specific questions students have on the reading materials. 2. Work through problems (conceptual, mathematical, or numerical) using “Clicker” questions and peer-to-peer instruction. I will randomly call students from the course roster (especially if I get insufficient voluntary participation). You should do all your reading with a journal available where you, among other things, list questions you have as you read. Once a section is completed, you should review the points you marked as unclear and formulate specific questions to ask me.

Assessment. The principal goal of assessment tools is to measure how well each student is realizing the course goals. I hope they will each provide a direct educational value to each student, including improvement in self-assessment skills.

A. In class participation and “clicker” questions. This includes a multiple-choice question based upon the reading assignment for that day. It will also include peer-learning questions. Note that each opportunity to vote will be counted for participation credit, but only the final vote (after you have had an opportunity to discuss the question) will count in terms selecting the correct answer. These will
be weighted as 30% of the final point total for the course. You will be allowed two absences from class during the term. Beyond that, you will receive zero credit for the points that could be earned during the class time on the missed days.

B. Problem Sets. Working through simple and complex calculations, often involving a combination of finding needed information, reducing the physical problem to a mathematical problem, and ultimately coming up with a numerical “answer” are essential skills that this course seeks for you to acquire. Perhaps more importantly, you will only achieve a deep understanding of the foundational concepts of the course if you translate these from abstractions to concrete, readily available tools that you will be able to intuitively use to solve tangible problems. There will be weekly problem sets due on Wednesdays, based upon material covered up to previous Friday’s readings, as well as material discussed in class up to that point. I encourage you to work in peer groups to solve these problem sets, but each student must submit his or her own work that they have written out. As you are writing out your own solution, make sure you understand where each input quantity and algebraic expressions came from, what approximations were made, and how the calculations were done. I encourage you to use Mathcad for solution of the problem sets. Many of the questions will require calculations, such as numerically solving differential equations or finding least square fits to data, that will not be practical to do on a hand calculator. Cumulatively, these problem sets will provide 30% of the final course point total.

C. Exams. There will be two in-term exams and a final exam. Exams will be cumulative as you will be asked to demonstrate that you can successfully integrate knowledge and skills learned in different parts of the course. The in-term exams will be two-part. There will be an in class written exam where you will be asked questions where you will have an opportunity to demonstrate your knowledge of the concepts of the subject, your ability to read diagrams, provide short answers to problems, and answer conceptual questions. The second part will taken out of class and will be presented as Mathcad documents that request you provide solutions to one or more problems similar to those you will encounter in the problem sets. In these cases, however, you will not be allowed to discuss the problems with your peers or reference other materials except those that I explicitly state you may. The final exam will be of the same format as the in-term exams but must be entirely completed during the University assigned exam period. Each in-class exam will be worth 10% of the total course points, and the final exam 20%. If you will not have personal access to a laptop that can run Mathcad during the final exam period, let me know sufficiently early in advance so I can arrange for you to borrow a laptop or do your exam in a computer lab.

Examination 1: Wednesday, October 3
Examination 2: Wednesday, November 7
Final Examination: Monday, December 10, 2-5 PM.
Web Materials: This course will use the Collab website 12F CHEM 3410-200 to post problem set assignments, reading assignments, course information, problem set solutions, etc. Most of the information will be in the Resources section under various headings. For critical issues, I will send an E-mail to the class. If you have not received an E-mail from me before the first day of class, please check your registration. If you have not already done so, you must acquire a I-clicker (version 1 is sufficient) and make its number is registered with your name so Collab can integrate with the I-Clicker software.