# **Department of Chemistry Courses**

## About Course Numbers:

Each Carnegie Mellon course number begins with a two-digit prefix that designates the department offering the course (i.e., 76-xxx courses are offered by the Department of English). Although each department maintains its own course numbering practices, typically, the first digit after the prefix indicates the class level: xx-1xx courses are freshmen-level, xx-2xx courses are sophomore level, etc. Depending on the department, xx-6xx courses may be either undergraduate senior-level or graduate-level, and xx-7xx courses and higher are graduate-level. Consult the Schedule of Classes (https://enr-apps.as.cmu.edu/open/SOC/SOCServlet/) each semester for course offerings and for any necessary pre-requisites or co-requisites.

## 09-052 Summer Internship

#### Summer: 3 units

The Department of Chemistry considers experiential learning opportunities important educational options for its undergraduate students. One such option is an internship, normally completed during the summer. Students do not need to officially register for an internship unless they want it listed on their official transcripts. The Director of Undergraduate Studies (or designee) will add the course to the student's schedule, and the student will be assessed tuition for 3 units. Upon completion of the internship, students must submit a 1-2 page report on their work experience to the Director of Undergraduate Studies (or other designated faculty member). Verification by the internship supervisor must be received prior to a grade being awarded. After the reports have been reviewed and approved, and verification received, a "P" grade will be assigned. Special permission of Instructor is required to register for this course.

## 09-101 Introduction to Experimental Chemistry

#### All Semesters: 3 units

This is a seven week chemistry laboratory course that is designed to introduce students to some basic laboratory skills, techniques, and equipment commonly used in experimental chemical investigations. The experiments will apply concepts in organic synthesis, quantitative analysis using visible spectrophotometry, kinetics, acid-base chemistry, thermochemistry, transition metal chemistry, and chromatography. 1 hr. lec., 3 hrs. lab.

## 09-103 Atoms, Molecules and Chemical Change

#### Fall: 9 units

Atoms, Molecules and Chemical Change is a self-contained one-semester introductory college chemistry course for students who have a high-school background in science and mathematics but who have decided not to major in a STEM field (science, technology, engineering, or mathematics). Students will develop fundamental chemical knowledge in topics such as stoichiometry, atomic theory, molecular bonding and structure, chemical reactions, thermodynamics, and electrochemistry. This knowledge will be applied to a variety of topics, including biological, industrial, environmental, agricultural, and culinary applications, helping students to understand how chemistry affects environmental, social, political, and economic issues. Through this course, students will develop both qualitative understanding and quantitative skills in chemistry. Students with credit for 09-105 or other more advanced chemistry courses are not permitted to enroll in this course. 3 hrs. lec., 1 hr. rec.

### 09-105 Introduction to Modern Chemistry I

#### Fall and Spring: 10 units

This course first investigates the establishment of some fundamental principles of chemistry and then progresses through the presentation of chemically interesting applications and sophisticated problems. It explores an understanding of matter and the energy changes associated with it, beginning with the atom. It then overviews how atoms interact and react to form the more complicated structures of molecules and ionic compounds How the structure of elements and compounds affects their properties, function, and reactivity will then be explored. Finally, the quantification of the changes during the reactivity of substances through bond breaking and forming will be investigated in single and multiple phase reactions, such as acid-base and redox reactions. Topics will be presented to promote mastery of "depth over breadth of topics" and "conceptual understanding before using applicable equations". The course covers the major principles of atomic structure, chemical bonding, , molecular structures of organic and inorganic compounds (including some transition metal complexes), interaction of substances, multiphase reaction stoichiometry, acid-base reactions, and redox reactions. Relevant examples will be drawn from such areas as environmental, materials, and biological chemistry.

## 09-106 Modern Chemistry II

#### Fall and Spring: 10 units

This course provides an overview of thermodynamics, kinetics and chemical equilibrium. Topics include the flow of energy in chemical systems; the spontaneity of chemical processes, i.e. entropy and free energy; the mechanisms and rates of chemical reactions; and the use of chemical equilibrium to reason about acid-base chemistry, solubility and electrochemistry. Applications include the energy economy, biological systems and environmental chemistry. 3 hrs. lec., 2 hrs. rec. Prerequisites: 09-105 or 09-107

## 09-107 Honors Chemistry: Fundamentals, Concepts and Applications

#### Fall: 10 units

This is an honors introductory course designed to provide students with a rigorous coverage of general chemistry in the context of grand challenges in the field. Traditional topics, such as equilibrium, kinetics, acid-base chemistry, and quantum chemistry, will be discussed through current research on nucleic acid-based therapeutics, atmospheric chemistry of pollutants, and catalysts for the production of solar fuels. The approach will integrate traditional lectures and readings from the textbook with discussions of journal articles, on-line content on research methods, and guest lectures from CMU faculty in these areas. This course assumes strong preparation in chemistry (AP Chemistry score of 3 or greater; IB Chemistry score of 5 or greater; SAT II Chemistry exam with a score of 700 or greater) and will be offered at an accelerated pace. The goal is to teach core principles of chemistry while exposing students to the diversity of modern chemical research and how it is addressing grand challenges facing society. 3 hrs. lec., 2 hrs. rec.

## 09-108 The Illusion and Magic of Food

#### Fall: 6 units

Have you ever wondered about your food? Why the freshly squeezed orange juice spoils after few hours while the one from the market lasts so much longer without apparent alteration? Why roasted food is so delicious? What is the nutritional value of milk and honey? Why soft drinks are damaging the teeth? What is the Impossible Burger? These and many more questions will be answered in this course, not only by the instructor but also through the student's research and curiosity. This course will introduce chemistry concepts on an as-needed basis, but it will remain at a simple level. We expect to help the student understand what food is made of, its nutritional value, how it is processed to offer longer shelf life, and how elaboration and preservation procedures may affect critical components. The topics will vary depending on the student's motivation in learning about different concepts related to the food industry, from processing to analysis, to packaging, and appearance. We plan to discuss interesting things in every class and finish the course with a broad knowledge of what is on our table and a better criteria to select our food. 3 hrs. lectures per week.

## 09-109 Kitchen Chemistry Sessions

## Intermittent: 3 units

Ever wanted to boil water in ice? Cook an egg so the yolk is set but the white still runny? Lick a lemon or drink vinegar but have it taste sweet? Make "caviar" from fruit juice and noodles from yogurt? Explore the science of molecular gastronomy through the lectures and demonstrations that reveal the chemistry and biochemistry of food ingredients and their preparation. Then use a kitchen as your "laboratory" to test hypotheses and delve into molecular cooking - you may just get to eat your lab results. For this course high school background in chemistry would help but nothing more advanced is required. Concepts will be discussed on a need to know basis. Students with stronger chemistry backgrounds should enroll in 09-209. 3 hrs. lec. and lab

## 09-110 The Design and Making of Skin and Hair Products

## Spring: 3 units

This hands-on course targets students from across the CMU community who are interested in learning how chemistry applies to their everyday life. We will focus on students gaining knowledge of the chemical components in cosmetic products and on the methods for preparing them (from shampoos and conditioners to lotions, soaps, and creams). We will emphasize good laboratory practices and safety as well as the fundamental chemical and physical concepts that govern the product behavior and use. The overarching goal is that the students have a hands-on laboratory experience and develop a full understanding of the science behind the products that they use every day. No human or animal testing will take place as part of the curriculum.

## 09-111 Nanolegos: Chemical Building Blocks

#### Fall: 9 units

How does chemistry provide the foundation and building blocks in science, engineering, and technology? How does activity on the particle and molecular level that we cannot see cause things to happen and function on a level we CAN observe? What basic chemical concepts are needed as tools to understand current significant research and technology, as well as to understand phenomena and problems in the world around us? This course will emphasize answering these questions by presenting "problem-or context-first", then applicable chemical concepts on an as-needed basis. It is structured around phenomena relevant to modern society, research, and technology rather than the conceptual tools (i.e. systemsor application-, rather than content-driven). Many of the conceptual tools (e.g. structure, interaction between energy and matter, interparticle forces, reaction stoichiometry, thermodynamics and kinetics) are used throughout the course, to help reinforce these ideas and promote an integrated understanding. The major contexts and phenomena that we will explore in applying and connecting chemical concepts are: (1) sustainable energy, (2) charge motion in materials, (3) natural versus engineered catalysts, (4) polymeric materials, and (5) reversible reactions in environmental and biological chemistry

## 09-114 Basics of Food Science

#### All Semesters: 3 units

Food is essential for life and the maintenance of health. As consumers we know little about its constitution and processing. This course will shed light upon the main nutrients found in food and their properties. We will discuss the importance of different processing techniques and about the ingredients added to food that extend its shelf life, or that improve its mouthfeel, and appearance. Overall, this course aims to make students aware of the intrinsic value of food, and how its manipulation and eventual reconstitution leads to an acceptable final product found in the supermarket.

## 09-115 Introduction to Undergraduate Research in Chemistry

## Fall: 2 units

Undergraduate research is an important activity in the training of undergraduate chemistry majors. This course is intended for students who are planning to declare a major in chemistry who are novices to research at the university level and have an interest in being better informed about strategies and skills that contribute to success. It is intended that this course will lead to an opportunity to participate in a series of shadowing opportunities through a second course in the spring semester where students will be mentored by upperclass students or PhD candidates in faculty laboratories. Spaces will be reserved for MCS students. Students from other colleges with a strong interest in a chemistry major or additional major should contact the Director of Undergraduate Studies in the Chemistry Department.

## 09-116 Undergraduate Research Shadowing in Chemistry

## Spring: 2 units

This is a follow-up course to 09-115, Introduction to Undergraduate Research in Chemistry, which is intended to provide laboratory training for first-year MCS students who want to participate in research in chemistry as soon as their first year, but have not been through the teaching labs yet. Near the end of the fall mini for 09-115, students will be asked to rank their faculty/group interests for possible shadowing. Based on those rankings and faculty/mentor availability, in 09-116, students will be paired with mentors from research labs for seven-week shadowing experiences. Mentors may be graduate students or advanced undergraduate students carrying out research. At the beginning of each mini, the students and mentors will identify blocks of time each week for shadowing based on their schedules. If scheduling allows, students will also be encouraged to attend group meetings (this would count toward lab time). Shadowing will continue for seven weeks, at which time the students may rotate to a second group for another shadowing experience. We request a dedicated lecture room to ensure there is adequate space for the initial pairing and for an overview on assessments, and to allow for possible additional meetings as the course develops.

Prerequisite: 09-115 Min. grade C

#### 09-122 Molecular Tools for Biological and Chemical Studies

#### Spring: 6 units

Fluorescent dyes are applied in numerous fields to aid in tasks such as mapping the course of water underground, examining the eye, and detecting biological events. This course is aimed at offering a handson laboratory experience in the interface of chemistry and biology, also known as bioorganic chemistry. In this lab students will learn about fluorescence and fluorescent compounds. They will prepare a dye and will measure its fluorescent properties in presence of different media. This behavior will be compared and contrasted with that of another dye that will be provided. A former student in the course says: "Molecular Tools for Biological and Chemical Studies was one of the highlights of my time at CMU! Taking this course during my freshman year allowed me to gain skill and confidence in the lab, and the concepts I learned helped me to excel in many other courses I took at CMU (including: Organic Chemistry I and amp; II, Laboratory I: Introduction to Chemical Analysis, Laboratory II: Organic Synthesis and Analysis, Biochemistry, and Modern Analytical Instrumentation). Since graduating from CMU, I have been working on a Ph.D. in chemical biology. I still use many of the skills that I learned in Molecular Tools on a daily basis." Maddie Balzarini

## 09-201 Undergraduate Seminar I

#### Fall: 1 unit

Issues and topics of importance to beginning chemistry majors are discussed in this course. It provides a general introduction to the facilities, faculty and programs of the Department of Chemistry and introduces students to career and research opportunities in the field of chemistry. Enrollment limited to students majoring in chemistry. 1 hr.

## 09-202 Undergraduate Seminar II: Safety and Environmental Issues for Chemists

#### Spring: 1 unit

Issues and topics focused on laboratory safety are discussed in this class. The topics are selected to supplement information covered in 09-221, Laboratory I. This course is intended to provide the necessary safety training for students wishing to undertake undergraduate research projects in the laboratory and is taught in collaboration with the Office of Environmental Health and Safety. Enrollment is limited to chemistry majors. 1 hr.

## 09-204 Professional Communication Skills in Chemistry

#### Spring: 3 units

This required course for chemistry majors promotes development of written and oral communication skills in various formats within the discipline. Students are expected to develop these skills by becoming more familiar with the style and format of the chemical literature, current topics in chemistry, and research projects in the Department. Other learning outcomes include developing critical reading skills, providing effective feedback to peers' written and oral communication, demonstrating the ability to revise written work, and using chemical structure drawing software. 1 hr. lec.

Prerequisite: 09-221

## 09-207 Techniques in Quantitative Analysis

## Fall: 9 units

09-207 is the first of two chemistry lab courses required for the BS and BA degrees in biological sciences and the intercollege major in biological sciences and psychology. It is also suitable for fulfilling the requirement for two general chemistry labs for admission to programs in the health professions. The experimental work emphasizes the techniques of quantitative chemical analysis. Included are projects dealing with a variety of instrumental and wet chemical techniques. A mixture of individual and partner experiments are conducted during the semester. In addition to laboratory techniques, safety, and written communication skills are emphasized.

Prerequisites: 09-107 Min. grade A or 09-106

#### 09-208 Techniques for Organic Synthesis and Analysis

#### Intermittent: 9 units

09-208 is the second of two chemistry laboratory courses required for the BS in biological sciences and the intercollege major in psychology and biological sciences. It is also suitable for fulfilling the requirement for the laboratory experience for application to programs in the health professions. The course emphasizes experimental work in separations, synthesis, and analysis of organic compounds, including chromatography and spectroscopy. Written communication skills will be developed by means of laboratory reports and essays. 1.5 hr lec, 5 hrs lab Prerequisites: (09-217 or 09-219) and (09-221 or 09-207 or 09-223)

## 09-209 Kitchen Chemistry Sessions

## Intermittent: 3 units

Ever wanted to boil water in ice? Cook an egg so the yolk is set but the white still runny? Lick a lemon or drink vinegar but have it taste sweet? Make "caviar" from fruit juice and noodles from yogurt? Explore the science of molecular gastronomy through the lectures and demonstrations that reveal the chemistry and biochemistry of food ingredients and their preparation. Then use a kitchen as your "laboratory" to test hypotheses and delve into molecular cooking - you may just get to eat your lab results. Students enrolling in this course are assumed to have a college level background in chemistry including introductory organic chemistry. Students without a solid chemistry background should take the lower level 09-109. 3 hrs. lec. and lab

Prerequisites: 09-219 or 09-217

## 09-214 Physical Chemistry

## Spring: 9 units

This is a one-semester course intended primarily for students majoring in Biological Sciences, students pursuing a B.A. degree program in Chemistry, and students in the B.S.A.program with a concentration in chemistry. The course focuses on thermodynamics, transport and reaction rates and their application to chemical and biological systems. Emphasis is given to attaining a good fundamental understanding of entropy and free energy. This is more a concepts than skills building course. Topics include applications of thermodynamics to chemical and biochemical equilibria, electrochemistry, solutions, and chemical kinetics. 3 hrs. lec. Prerequisites: 09-106 and (21-122 or 21-124) and (33-141 or 33-121 or 33-111 or 33-106)

## 09-215 Chemistry Tech I to Lab I Transition

## Fall and Spring: 3 units

09-215 is a 3-unit course intended for students who have taken 09-207, Techniques in Quantitative Analysis, who decide later in their academic experience that they wish to pursue a degree or an additional major in chemistry. The chemistry major requires a 12-unit lab class, 09-221 Laboratory I: Introduction to Chemical Analysis. This course will utilize selfstudy and problem solving to introduce or reinforce key concepts covered in 09-221 that are not introduced or are de-emphasized in 09-207. Students will also propose an idea for an independent lab-based project and carry it through all stages of development but not perform the actual lab work. The project development will require written work products as well as an oral presentation. The course must be completed before the last semester of the students degree program.

Prerequisite: 09-207 Min. grade C

## 09-216 Chemistry Tech II to Lab II Transition

#### Fall: 3 units

09-216 is a 3-unit course intended for students who have taken 09-208, Techniques in Organic Synthesis and Analysis, who decide later in their academic experience that they wish to pursue a degree or an additional major in chemistry. The chemistry major requires a 12-unit lab class, 09-222 Laboratory II: Organic Synthesis and Analysis. This course will utilize selfstudy and problem solving to introduce or reinforce key concepts covered in 09-222 that are not introduced or are de-emphasized in 09-208.

## 09-217 Organic Chemistry I

#### Fall: 9 units

This course presents an overview of structure and bonding as it pertains to organic molecules. Selected topics include: introduction to functional group chemistry, stereochemistry, conformational analysis, reaction mechanisms and use of retrosynthetic analysis in the development of multistep syntheses. Methods for structure determination of organic compounds by modern spectroscopic techniques are introduced. 3 hrs. lec., 1 hr. rec.

Prerequisites: 09-105 or 09-107

## 09-218 Organic Chemistry II

#### Spring: 9 units

This course further develops many of the concepts introduced in Organic Chemistry 1, 09-217. Emphasis is placed on the utilization of reaction mechanisms for understanding the outcome of chemical transformations, and the employment of a wide variety of functional groups and reaction types in the synthesis of organic molecules. Also included in the course will be special topics selected from the following; polymers and advanced materials, biomolecules such as carbohydrates, proteins and nucleic acids, and drug design. 3 hrs. lec., 1 hr. rec. Prerequisites: 09-217 or 09-219

#### 09-219 Modern Organic Chemistry

#### Fall: 10 units

Traditional introductory organic chemistry courses present structure, reactivity, mechanisms and synthesis of organic compounds. Students taking 09-219 will be exposed to the same topics, but presented in greater depth and broader context, with applications to allied fields such as (1) polymer and materials science, (2) environmental science and (3) biological sciences and medicine. This will be accomplished through an extra 50 minute lecture period, where more advanced topics and applications will be discussed. Topics will include computational chemistry, green chemistry, chiral separations, photochemistry, reaction kinetics, controlled radical polymerizations and petroleum cracking. Students who complete 09-219 will have a strong foundation in organic chemistry as well as a sophisticated understanding of how organic chemistry is currently practiced. 4 hrs. lec., 1 hr. rec.

Prerequisites: 09-106 or 09-107 Min. grade A

## 09-220 Modern Organic Chemistry II

## Spring: 10 units

This course builds on 09-219 by introducing students to additional functional groups, chemical reaction mechanisms and synthetic strategies commonly used in the practice of organic chemistry. Advanced topics to be presented during the extra lecture will include multidimensional NMR spectroscopy, enantioselective synthesis, ionic polymerization, bioorganic and medicinal chemistry, natural products chemistry and toxicology. Students who complete 09-220 will have a strong foundation in synthetic, mechanistic and structural organic chemistry and will understand how this applies to human health and the environment. 4 hrs. lec, 1 hr. rec. Prerequisite: 09-219

## 09-221 Laboratory I: Introduction to Chemical Analysis

#### Fall and Spring: 12 units

This course is the first in a sequence of four laboratory courses on experimental aspects of chemistry required for the B.S. and B.A. degrees in chemistry. The experimental work emphasizes the techniques of quantitative chemical analysis. Included are projects dealing with a variety of instrumental and wet chemical techniques. The course is project-oriented with the experiments becoming more complex, requiring greater student input into the experimental design as the semester progresses. A mixture of individual and team experiments are conducted during the semester. In addition to techniques, safety, written and oral communication skills, and effective teamwork are emphasized. 2 hrs. lec., 6 hrs. lab. Prerequisites: 09-106 or 09-107 Min. grade A

## 09-222 Laboratory II: Organic Synthesis and Analysis

Fall and Spring: 12 units

In this second course in the laboratory sequence, students acquire laboratory skills relevant to synthesis and purification of organic compounds, as well as the practical use of chromatography and spectroscopy. Students will also further develop technical writing skills through preparation of lab reports. 2 hrs. lec., 6 hrs. lab. Prerequisites: (09-219 or 09-217) and (09-223 or 09-221)

#### 09-224 Supramolecular Chemistry

## Intermittent: 3 units

Supramolecular chemistry involves the use of noncovalent bonding interactions to assemble molecules into stable, well-defined structures. This course will provide students with an introduction to this exciting field of research, which is finding increasing applications in the biological and materials sciences, nanotechnology and medicine. Students will be introduced to essential background concepts such as types of noncovalent bonding and strategies for the design of supramolecular assemblies. Readings from monographs and classroom lectures by the instructor will cover this material. Students will then begin to read about applications of supramolecular chemistry from the scientific literature, learning to compare articles, to evaluate the quality of the data and interpretations reached by the authors, to use the knowledge gained from these readings and discussions to predict the outcomes of related experiments, and to ultimately be able to design their own experiments to answer research questions. Meeting hours set by instructor, enrollment limited with priority given to sophomore chemistry majors.

Prerequisites: 09-219 Min. grade C or 09-217 Min. grade C

## 09-225 Climate Change: Chemistry, Physics and Planetary Science

## Fall: 9 units

Understanding the essential features of climate and climate change is a critical tool for modern citizens and modern scientists. In addition, the prevalence of climate skepticism in modern political discourse requires of citizens that they be able to think critically about a technical subject and also be able to distinguish reliable scientific experts from advocates. In this course we shall examine the climate of terrestrial planets (specifically Earth and Venus) through geological time and to the present, considering geochemical methods used to determine atmospheric composition over Earths history (specifically the onset of oxygen in the atmosphere as well as the relationship between carbon dioxide and global temperature over geological timescales. The shorter climate history of Venus will be considered as a counter example, where the brightening dim young sun overwhelmed negative feedbacks in the weathering cycle, leading to a runaway greenhouse amplified by complete evaporation of the onetime Venus ocean. Throughout the course, we will consider climate change driven by human activity since the industrial revolution as a unifying theme. Prerequisites: (09-107 or 09-105) and (33-141 or 33-121 or 33-151)

## 09-227 The Culture of Color: Dyes, Chemistry, and Sustainability

#### All Semesters: 9 units

ne of the earliest forms of proto-chemistry, dyeing textiles has a long history of rich cultural traditions and technical innovations - which we will explore and practice. In this course students will focus on color through working with dyes for textiles scientifically, artistically, and culturally. You will learn the chemical science of color and techniques to isolate natural pigment for dyes as well as how to produce dyes synthetically. Students learn a variety of methods to apply our dyes to textiles to create beautiful patterns: immersion dyeing, resist and folding techniques, and printing. You will be exposed to the use of laboratory equipment and will be trained in good laboratory practices and safety. In preparation for your final project, throughout the course, we will discuss the cultural significance of colors, the origin of pigments, their production impact on the economy of the area, sustainability, and environmental impact of the waste produced by the textile dyeing industry.

Course Website: http://www.chem.cmu.edu/

## 09-231 Mathematical Methods for Chemists

#### Fall: 9 units

This course uses mathematical approaches to develop models for chemical systems and materials from the bottom up, i.e. from atoms and molecules to substances. This course focuses on statistical mechanics and does not cover quantum mechanics basics. Math will be covered in the context of chemical phenomena, and combine topics from probability theory and statistics, 3-dimensional calculus, differential equations, and linear algebra. 3 hrs. lec.

Prerequisites: (09-107 Min. grade A or 09-106) and (21-124 or 21-122)

## 09-291 Environmental Systems on a Changing Planet

## Fall: 9 units

This course introduces the interconnected environmental systems that regulate our climate and ecosystems, providing the resources required to sustain all life, including human societies. These systems are the fascinating connections between the oceans, atmosphere, continents, ecosystems, and people that provide our planet with resources that all life depends on. Human activities disrupt these natural systems, posing critical threats to the sustainable functioning of environmental systems. We will explore how solar and biochemical energy moves through the Earths interconnected systems, recycling nutrients; how complex environmental systems function to produce critical resources such as food and water; and how human activities interfere with these systems. Case studies include the interplay between climate change feedbacks, wildfires, and forest ecosystems; the hazards that everyday chemical toxins pose to ecosystems and human health and reproduction; and growing threats to ecosystem health and biodiversity. We will also develop the relevant information literacy required to understand current issues that are frequently debated in the public sphere, and connect these to environmental justice. This course draws on principles learned in high school science and serves as the foundational Barth and amp; Environmental Science requirement for both the Minor and Additional Major in Environmental and Sustainability Studies. 09-291 is intended for both non-STEM majors from any program as well as STEM majors from any program in CIT, MCS, and SCS. In addition, STEM majors are strongly encouraged to take the connected 09-381 3-unit course that provides a more technical and quantitative framework for understanding the course content. 24-381 is often required for this course to count as a technical elective for STEM programs, and is required for students from CIT, MCS, and SCS in the Environmental and Sustainability Studies programs.

## 09-301 Undergraduate Seminar III

#### Fall: 1 unit

Students attend seminars on current topics in chemistry. Students are sent a menu of choices for each week of the semester and may select topics of interest. Enrollment is restricted to students majoring in chemistry. 1 hr.

#### 09-302 Undergraduate Seminar IV

#### Spring: 1 unit

Students attend seminars presented by senior chemistry majors. Students provide peer evaluations of the seminars and through the process students become familiar with special topics in chemistry. The course establishes what should be included in a good seminar. This seminar courses is one of 6 required for the chemistry major. If a schedule conflict exists, students may, with permission of the instructor, attend other chemistry seminars or make other arrangements to fulfill the requirement. 1 hr.

#### 09-303 Hooked: The Molecular Basis of Addiction

#### Fall: 6 units

What makes us need something so much that it eclipses the most important aspects of our lives, such as family, friends, work, hobbies, health and wellness? There are many different types of addiction; this course will focus on molecular addictions, with an emphasis on those involving members of the opioid class of narcotics. The ongoing epidemic of opioid addiction, arising both from over-prescription of pain killers and recreational use of heroin, has been widely reported and continues to rise at alarming rates, ravaging our urban and rural communities. In this course, we will explore the complicated role of chemistry in this epidemic, including the good (elucidating mechanisms of action, developing clinically useful and safe opioids and non-opioids) and the bad (design and synthesis of by the pharmaceutical industry that prescribes them, the government agencies charged with regulating these activities and law enforcement agencies that attempt to stop the flow of drugs into and within the United States. The second half of the semester will focus on addiction to other drugs, including cocaine, marijuana, amphetamines, alcohol and nicotine. We will also discuss chemical approaches to treating addiction. Students who complete this course will emerge with a broad understanding and perspective on an issue that is of great scientific and societal importance. The course will be organized in units that begin with a historical/societal "big picture" overview, followed by technical discussions of the underlying chemistry and biochemistry, concluding with consideration of the societal implications of addiction to each particular substance.

## 09-321 Laboratory III: Molecular Design and Synthesis

## Fall: 12 units

In this third course in the laboratory sequence, students will learn a variety of more advanced techniques for organic synthesis and characterization, and will gain experience with developing and designing synthetic procedures. Student writing skills are further reinforced through preparation of detailed lab reports. 2 hrs. lec., 6 hrs. lab. Prerequisites: (09-220 or 09-218) and 09-222

## 09-322 Laboratory IV: Molecular Spectroscopy and Dynamics

## Spring: 12 units

This laboratory course is devoted to physical chemistry experiments, which involve the use of modern spectroscopic instrumentation to probe the optical and magnetic properties of molecules. The experiments include the use of high-resolution infrared, laser Raman, NMR, EPR, fluorescence, and UV-visible spectroscopies. Additional experiments demonstrate methods for measuring enzyme-catalyzed reaction rate constants, and the use of scanning probe microscopy for imaging and characterization of biological macromolecules. Throughout the course the students will learn how to use computer algebra packages for rigorous data analysis and modeling and will develop the skills in basic electronics, and vacuum techniques. 2 hrs. lec., 6 hrs. lab.

Prerequisites: (09-221 or 09-223) and 09-344

#### 09-323 Bioorganic Chemistry Laboratory

## 12 units

Bioorganic chemistry is concerned with the action of synthesized compounds on biological systems. In order to maximize the likelihood of identifying a biologically active compound, synthetic libraries are often employed, requiring extensive familiarity with simple, efficient chemical coupling steps and protecting group chemistry. In this inquiry based laboratory course, using a process that mimics the current practice in drug discovery by pharmaceutical companies, students will rationally design a compound library in hopes of finding a compound active against a selected biological target, search for active compounds in the library, and then quantitatively characterize any identified compounds for activity. Working in small groups, students will develop proposals for and execute the target assay selected, the library synthesis, and the screening approach. Students will write reports summarizing the results in each phase of the course. Throughout the course, students will be introduced to concepts relevant to industrial scientific research, including regulatory compliance, quality control and assurance, and intellectual property. Prerequisites: (09-218 or 09-220) and 09-222

## 09-325 Special Topics in Chemistry: Environmental Systems on A Changing Planet

#### All Semesters: 9 units

This course introduces the interconnected Earth systems that regulate our climate and ecosystems, providing the resources required to sustain all life, including human societies. Environmental systems are the fascinating connections between the oceans, atmosphere, continents, ecosystems, and people that provide our planet with resources that all life depends on. Human activities disrupt these natural systems, posing critical threats to the sustainable functioning of environmental systems. The course will explore how solar and biochemical energy moves through the Earth's interconnected systems, recycling nutrients; how complex environmental systems function to produce critical resources such as food and water; and how human activities interfere with environmental systems. Case studies include the interplay between climate change feedbacks, wildfires, and forest ecosystems; the hazards that everyday chemical toxins pose to ecosystems and human health and reproduction; and growing threats to ecosystem health and biodiversity. We will also develop the environmental, scientific, and information literacy required to understand current environmental issues that are frequently debated in the public sphere. This course draws on principles learned in high school science and satisfies the science requirement for the interdisciplinary Minor in Environmental and Sustainability Studies.

## 09-331 Modern Analytical Instrumentation

#### Fall: 9 units

This course will cover all aspects of analytical instrumentation and its application to problems in materials, environmental, and biological chemistry. Topics covered will include mass spectrometry, optical spectroscopies and NMR. In addition, the course will emphasize how to select an analytical method appropriate to the problem at hand, how to optimize the signal to noise obtained by a measurement, and the quantitative analysis of experimental data. Some basic electronics will be covered as well. 3 hrs. lec.

## 09-344 Physical Chemistry (Quantum): Microscopic Principles of Physical Chemistry

#### Fall: 9 units

We will connect your qualitative understanding of atoms and molecules to a more quantitative treatment, so that each of you can independently assess the extent to which chemistry is based on fundamental principles. To do this we must study the basic principles of quantum theory, because atoms and molecules are quantum particles. These principles influence every aspect of how you think of chemistry and the course will challenge you to think in different ways about the stuff around you. Throughout the course we shall apply quantum principles to develop an understanding of molecular and atomic spectroscopy, and a concurrent understanding of how spectroscopy can be used to learn about the microscopic properties of atoms and molecules. 3 hrs. lec., 1 hr. rec.

Prerequisites: (09-105 or 09-107) and (33-121 or 33-151 or 33-106 or 33-111 or 33-141)

## 09-345 Physical Chemistry (Thermo): Macroscopic Principles of Physical Chemistry

#### Spring: 9 units

The measurement and theoretical descriptions of the equilibrium properties of chemical systems are presented. Chemical thermodynamics is introduced at the upper division level. The phases of matter are discussed. The quantitative treatment of mixtures is developed. The detailed description of chemical equilibrium is elaborated. The measurement and theoretical description of the nonequilibrium properties of chemical systems are presented. Elementary transport properties are introduced. The principles of classical chemical kinetics are developed in great detail. 3 hrs. lec., 1 hr. rec.

Prerequisites: (09-106 or 09-107) and (21-259 or 09-231)

## 09-348 Inorganic Chemistry

#### Spring: 10 units

The focus of this class is understanding the properties of the elements and of the inorganic compounds. The electronic structure of elements is discussed as the basis for the element's organization in the Periodic Table and for their properties. We will discuss atomic structure, and bonding of diatomic and polyatomic molecules using different models such as Lewis structures, VSEPR and Molecular Orbital Theory (including group theory and linear combination of atomic orbitals). We will study the structure, spectroscopy, and reactivity of coordination complexes and their application in bioinorganic and organometallic chemistry. 3 hrs. lec., 1 hr. rec. Prerequisites: (09-107 or 09-105) and 21-120

## 09-381 Environmental Systems on a Changing Planet

## Fall: 12 units

This is 3-unit addendum to the co-requisite 09-291: Environmental Systems on a Changing Planet. These courses introduce the interconnected Earth systems that regulate our climate and ecosystems, providing the resources required to sustain all life and human societies. Please refer to the course description for 09-291 for more information. While 09-291 is designed to be accessible to students from all Colleges and majors, this addendum allows students to engage with the material with more technical depth and quantitative understanding of the function and feedbacks of complex environmental systems. The additional 3-units of 09-381 provides students with an additional weekly meeting time for further material development and discussion, and with additional assignments and exercises on top of 09-291. 09-381 is intended for students from STEM majors in CIT, MCS, and SCS, but can be taken by any student interested in exploring the environmental science topics with greater depth. Science and engineering fundamentals will be further developed and applied to develop the quantitative understanding of the function and feedbacks of complex environmental systems. A background in the natural sciences or engineering (such as introductory-level courses) is strongly recommended for students considering taking 09-381. When taken with 09-291, 09-381 will count as a technical elective for most programs in these STEM colleges, while 09-291 on its own is not considered a technical elective. 09-381 with 09-281 is the correct course for students whose home colleges are CIT, MCS, or SCS. 09-291 is the recommended course for students whose home colleges are CFA, DC, or TBS. 09-381 with 09-291 serve as the foundational Earth and amp; Environmental Science requirement for STEM majors for both the interdisciplinary Minor and Additional Major in Environmental and Sustainability Studies.

## 09-401 Undergraduate Seminar V

#### Fall: 1 unit

Students attend seminars on current topics in chemistry. Students are sent a menu of choices for each week of the semester and may select topics of interest. Enrollment is restricted to students majoring in chemistry. 1 hr.

## 09-402 Undergraduate Seminar VI

#### Fall and Spring: 3 units

Students enrolled in this course present a 20 - 30 minute oral report on a current topic in chemistry. This may be from the student's research work or a special chemistry topic of general interest. Presentations or papers prepared for other courses are not acceptable for this purpose. Thoroughness in the use of the chemical literature is emphasized. The use of presentation aids such as PowerPoint is required. Other students in the class submit written evaluations of the presentation. Talks are recorded for viewing by the student and instructor as a means of providing individualized feedback about presentation skills. A seminar presentation is required of all chemistry majors. No exceptions possible. Enrollment is limited to students majoring in chemistry. 1 hr.

## 09-403 Hooked: The Chemical Basis of Drug Addiction

#### Fall: 9 units

What makes us need something so much that it eclipses other important aspects of our lives, such as family, friends, work, hobbies, health and wellness? There are many different types of addiction; this course will focus on molecular addictions, specifically those involving members of the opiate class of narcotics. The ongoing epidemic of opiate addiction, arising both from over-prescription of pain killers and recreational use of heroin, has been widely reported and continues to rise at alarming rates, ravaging our urban and rural communities. In this course, we will explore the complicated role of chemistry in this epidemic, including the good (elucidating mechanisms of action, development of clinically useful and safe opiates and non-opiate pain killers) and the bad (design and synthesis of increasingly addictive opiates). We will also discuss ethical questions faced by the pharmaceutical industry that develops, markets and sells opiates, the medical community that prescribes opiates, students who complete this course will emerge with a broad understanding and perspective on an issue that is of great scientific and societal importance. 3 hrs. lec. Prerequisites: 09-218 or 09-220

## 09-425 Special Topics in Chemistry:Environmental Exposure and Risk Assessment

#### All Semesters: 9 units

Our world is full of synthetic and naturally occurring toxic chemicals, presenting an imminent but difficult-to-quantify threat for human and ecosystem health. In this papers-based course we will ask the question, "How do we decide what's 'safe'?" in the context of exposure and risk assessment for toxic environmental pollutants. We will complete a series of case studies featuring current and seminal literature, in-class activities, and project-based assignments. Each case study will focus on a distinct contaminant exposure scenario and will be linked back to the common theme of using chemistry to understand how external exposure leads to internal dose and subsequent health impacts for diverse environmental pollutants. We will discuss how knowledge generated in the laboratory can be translated and used to inform regulatory decisions. The first half of the course will focus on contaminant bioavailability, exposure, and toxic effects in aquatic organisms. In the second half of the course, we will discuss human exposure to toxic pollutants and strategies to assess risks in the human population, including the human exposome concept, -omics-based research, and strategies for discovering novel harmful contaminants. Prerequisites: (09-106 or 09-107) and (09-217 or 03-232 or 09-219 or 03-231)

## 09-435 Independent Study Chemistry

#### All Semesters

The course allows students to earn academic credit for concentrated study in a topic area developed in conjunction with and monitored by a faculty member in the Department of Chemistry. These topics are distinct from projects that would rise to the level of undergraduate research either because they are in unrelated areas distinct from the faculty member's research interests or may constitute the investigation and compilation of existing information from a variety of resources and may not be expected to result in the generation of new information as is a reasonable expected outcome in undergraduate research (likely is not publishable).

## 09-445 Undergraduate Research

## Fall and Spring

Properly qualified students may undertake research projects under the direction of members of the faculty, normally 6 to 12 hrs/week. A written, detailed report describing the project and results is required. Course may be taken only with the consent of a faculty research advisor in chemistry or on occasion in another department provided that the project is chemical in nature and with permission of the Director of Undergraduate Studies. The number of units taken generally corresponds to the actual number of hours the student actually spends in the lab doing research during the week. Maximum number of units taken per semester is 18.

#### **09-455 Honors Thesis**

## Fall and Spring

Students enrolled in the departmental honors program (B.S. with Departmental Honors or combined 4-year B.S./M.S. degree) are required to enroll in this course to complete the honors degree requirements. A thesis written in an acceptable style describing an original research project, and a successful oral defense of the thesis topic before a THesis Committee are required. Limited to students accepted into the honors program. (B.S. Honors candidates normally enroll for 6 units; B.S./M.S. candidates enroll for 15 units.)

## 09-502 Organic Chemistry of Polymers

#### Spring: 9 units

A study of the synthesis and reactions of high polymers. Emphasis is on practical polymer preparation and on the fundamental kinetics and mechanisms of polymerization reactions. Topics include: relationship of synthesis and structure, step-growth polymerization, chain-growth polymerization via radical, ionic and coordination intermediates, copolymerization, discussions of specialty polymers and reactions of polymers. 09-509, Physical Chemistry of Macromolecules, is excellent preparation for this course but is not required. 3-6 hrs. lec. (Graduate Course: 12 units, 09-741)

Prerequisites: 09-220 or 09-218

#### **09-507 Nanoparticles**

## Intermittent: 9 units

This course discusses the chemistry, physics, and biology aspects of several major types of nanoparticles, including metal, semiconductor, magnetic, carbon, and polymer nanostructures. For each type of nanoparticles, we select pedagogical examples (e.g. Au, Ag, CdSe, etc.) and introduce their synthetic methods, physical and chemical properties, self assembly, and various applications. Apart from the nanoparticle materials, other topics to be briefly covered include microscopy and spectroscopy techniques for nanoparticle characterization, and nanolithography techniques for fabricating nano-arrays. The course is primarily descriptive with a focus on understanding major concepts (such as plasmon, exciton, polaron, etc.). The lectures are power point presentation style with sufficient graphical materials to aid students to better understand the course materials. Overall, this course is intended to provide an introduction to the new frontiers of nanoscience and nanotechnology. Students will gain an understanding of the important concepts and research themes of nanoscience and nanotechnology, and develop their abilities to pursue highly disciplinary nanoscience research. The course should be of interest and accessible to advanced undergraduates and graduate students in fields of chemistry, materials science, and biology. 3 hrs. lec.

## 09-509 Physical Chemistry of Macromolecules

#### Fall: 9 units

This course develops fundamental principles of polymer science. Emphasis is placed on physio-chemical concepts associated with the macromolecular nature of polymeric materials. Engineering aspects of the physical, mechanical and chemical properties of these materials are discussed in relation to chain microstructure. Topics include an introduction to polymer science and a general discussion of commercially important polymers; molecular weight; condensation and addition synthesis mechanisms with emphasis on molecular weight distribution; solution thermodynamics and molecular conformation; rubber elasticity; and the rheological and mechanical properties of polymeric systems. (This course is also listed as 09-715, 12 units) 3 hrs. lec.

### 09-510 Chemistry and Sustainability

#### Spring: 9 units

This course aims to educate students in the foundations of systematic leadership for building a sustainable world. Many sustainability challenges are associated with commercial chemicals and with operational modes of the chemical enterprise. For scientists, effectiveness in solving the technical challenges and redirecting cultural behavior is the defining substance of sustainability leadership. The course aims to challenge students to analyze and understand the root causes of unsustainability, especially in the technological and cultural dimensions of the chemical enterprise, to imagine a more sustainable world and to begin to define personal leadership missions. Students will be introduced to sustainability ethics as the foundation stone of transformative sustainability leadership, to the Collins Code of Sustainability Ethics and to other guiding tools. The Collins Bookcase of Green Science Challenges organizes the technical content. It systematizes the major chemical sustainability challenges of our time: clean synthesis, renewable feed-stocks, safe energy, elemental pollutants, persistent molecular toxicants and endocrine disruptors. Focal areas will be the technical, toxicological and cultural histories of elemental and molecular pollutants and endocrine disruptor (ED) science. EDs represent the single greatest sustainability challenge of everyday chemicals all while we are just beginning to recognize an emerging threat to health and the environment from micro- and nano-plastics which are finding their way into human tissues. The course is intended for upper level undergraduates and graduates, although many brilliant freshmen have thrived in the course. The class is limited to 25 students. The assignments are common to both undergraduate and graduate classes offerings with graduates taking additional assignments. (Undergraduate course 9 units 09-510. Graduate course 12 units 09-710) 3 hrs. lec.

## 09-517 Organotransition Metal Chemistry

#### Intermittent: 9 units

The first half of this course focuses on the fundamentals of structure and bonding in organotransition metal complexes and how the results can be used to explain, and predict, chemical reactivity. The latter half of the course covers applications, and more specifically, homogeneous catalysts for industrial processes and organic synthesis. (Graduate Course: 12 units, 09-717)

Prerequisite: 09-348

## 09-518 Bioorganic Chemistry: Nucleic Acids and Carbohydrates

#### Fall: 9 units

This course will introduce students to new developments in chemistry and biology, with emphasis on the synthesis, structural and functional aspects of nucleic acids and carbohydrates, and their applications in chemistry, biology and medicine. Later in the course, students will have the opportunity to explore cutting-edge research in this exciting new field that bridges chemistry with biology. Students will be required to keep abreast of the current literature. In addition to standard homework assignments and examinations, students will have the opportunity to work in teams to tackle contemporary problems at the forefront of chemistry and biology. The difference between the 09-518 (9-unit) and 09-718 (12-unit) is that the latter is a graduate level course. Students signed up for 09-718 will be required to turn in an original research proposal at the end of the course, in addition to all the other assignments. (Graduate Course: 12 units, 09-718) 3 hrs. lec.

Prerequisites: (03-121 or 03-151) and (09-220 or 09-218)

## 09-519 Bioorganic Chemistry: Peptides, Proteins and Combinatorial Chemistry

#### Spring: 9 units

This course will introduce students to new developments in chemistry and biology, with emphasis on the synthesis, structural and functional aspects of peptides, proteins and small molecules. Basic concepts of bioorganic chemistry will be presented in the context of the current literature and students will have the opportunity to learn about the experimental methods used in various research labs. An introduction to combinatorial chemistry in the context of drug design and drug discovery will also be presented. Students will be required to keep abreast of the current literature. Homeworks and team projects will be assigned on a regular basis. The homework assignments will require data interpretation and experimental design; and team projects will give students the opportunity to work in teams to tackle contemporary problems at the interface of chemistry and biology. Students enrolled in the graduate level course (09-719) will be required to turn in an original research proposal at the end of the course, in addition to the homework assignments, midterm, and final exam that are required for the undergraduate course. (Graduate Course: 12 units 09-719) 3 hrs. lec

Prerequisites: (03-151 or 03-121) and (09-218 or 09-220)

#### 09-521 Metals in Biology: Function and Reactivity

#### Intermittent: 6 units

Metal ions play important roles in many biological processes, including photosynthesis, respiration, global nitrogen cycle, carbon cycle, antibiotics biosynthesis, gene regulation, bio-signal sensing, and DNA/RNA repair, just to name a few. Usually, metal ions are embedded in protein scaffold to form active centers of proteins in order to catalyze a broad array of chemical transformations, which are essential in supporting the biological processes mentioned above. These metal containing proteins, or metalloproteins, account for half of all proteins discovered so far. In this course, the relation between the chemical reactivity and the structure of metalloproteins will be discussed in detail. The main focus is to illustrate the geometric and electronic structure of metal centers and their interactions with the protein environment in governing the chemical reactivity of metalloproteins. The applications of these principles in designing biomimetic/bioinspried inorganic catalysts and in engineering metalloproteins bearing novel chemical reactivity will also be discussed. The basic principles of the frequently utilized physical methods in this research area will also be introduced, which include optical absorption spectroscopy, Infrared (IR) and Raman spectroscopies, M and #246;ssbauer spectroscopy, electron paramagnetic resonance (EPR), X-ray absorption and diffraction techniques. Prerequisites: (09-344 or 09-345 or 09-214 or 09-347) and 09-348

#### 09-522 Kinetics and Mechanisms of Chemical and Enzymatic Reactions

## Intermittent: 9 units

This is a practical course aimed at learning the major modern tools which are essential for investigation of mechanisms of homogeneous chemical and enzymatic reactions. Rules of formal chemical kinetics in solution are first considered followed by basic principles of kinetics of enzymatic processes including inhibition, which is a key factor in the up-to-date drug design. The relationships between electronic structures, catalytic properties, and reactivity of biologically relevant metal complexes will be provided. Electrochemical and redox features of metal complexes will be reviewed. The course includes such hot topics as Fenton chemistry, Marcus's electron transfer concept, catalysis by Collins' TAML activators of peroxides, specific and general acid/base, proximal and micellar catalysis. Mechanistic pathways of action of hydrolases, kinases, hydrogenases, oxidases, peroxidases, cytochrome P-450, and other metalloenzymes will be described. The course is supplied by the recently published text (A. D. Ryabov "Practical Kinetics and Mechanisms of Chemical and Enzymatic Reactions" Cambridge Scholars Publishing, Newcastle upon Tyne, NE6 2PA, UK) which includes all the above mentioned themes (Graduate course: 09-722, 12-units) 3 hrs. lec. Prerequisite: 09-348 Prerequisite: 09-348

## 09-524 Environmental Chemistry

#### Spring: 9 units

Environmental pollutants are common consequences of human activities. These chemicals have a wide range of deleterious effects on the environment and people. This course will introduce students to a range of major environmental pollutants, with a particular focus on persistent organic pollutants. We will use chemical principles including thermodynamics, kinetics, photochemistry, organic reaction mechanisms, and structure activity relationships to understand the environmental fate of major classes of pollutants. The transport of chemicals through the environment and their partitioning between air, water, soil, and people will be described. The major environmental reaction pathways (oxidation, photolysis, hydrolysis, reduction, metabolism) of common pollutants will be explored. This will provide students with the necessary knowledge to predict the chemical fate of environmental pollutants, and improve their understanding of the environmental impacts of their everyday chemical use and exposure. Specific topics include water quality, photochemical smog, organic aerosols, atmospheric chemistry and global climate change, toxicity of pesticides, and heterogeneous and multiphase atmospheric chemistry. The 12-unit course is intended for graduate students that want to explore aspects of the course more deeply. This includes additional requirements including a final term paper and in-class presentation, and additional advanced questions on the homework assignments. Prerequisites: 09-219 or 09-217

## 09-525 Transition Metal Chemistry

## Intermittent: 9 units

This class is focused understanding the structure, spectroscopy and reactivity of 3d metal complexes. Based on ligand field theory, we will analyze the electronic structure of these metal complexes and we will briefly describe the main spectroscopic techniques that will allow for studying this topic (X-ray diffraction analysis, UV-vis, EPR, NMR, EXAFS and Mossbauer). The main focus of the course will be on analyzing the reactivity of 3d metal complexes in the context of metalloenzymes and small-molecule bioinspired complexes. The natural and synthetic metal complexes involved in O2 reduction, H2O oxidation, N2 reduction, H2 formation and functionalization of organic molecules (e.g. hydroxylation of C-H bonds, dehydrogenation of alcohols, etc.), and the reaction pathways by which these important processes take place will be studied in detail. (Graduate Course: 12 units, 09-725) 3 hrs. lec. Prereguisite: 09-348

## 09-529 Introduction to Sustainable Energy Science

#### Fall: 9 units

This course focuses on the chemistry aspects of sustainable energy science. It introduces the major types of inorganic and molecular materials for various important processes of energy conversion and storage, such as photovoltaics, fuel cells, water splitting, solar fuels, batteries, and CO2 reduction. All the energy processes heavily rely on innovations in materials. This course is intended to offer perspectives on the materials/physical chemistry that are of importance in energy processes, in particular, how the atomic and electronic structures of materials impact the energy harvesting and conversion. In current energy research, intense efforts are focused on developing new strategies for achieving sustainable energy through renewable resources as opposed to the traditional oil/coal/gas compositions. This course offers students an introduction to the current energy research frontiers with a focus on solar energy conversion/ storage, electrocatalysis and artificial photosynthesis. The major types of materials to be covered include metals, semiconductors, two-dimensional materials, and hybrid perovskites, etc. The material functions in catalysis, solar cells, fuel cells, batteries, supercapacitors, hydrogen production and storage, realso discussed in the course. The lectures are power-point presentation style with sufficient graphical materials to aid students to better understand the course materials. Demo experiments are designed to facilitate student learning

Prerequisites: (09-107 or 09-105) and (33-121 or 33-141 or 33-151)

#### 09-530 Chemistry of Gene Expression

#### Fall: 9 units

This course examines the chemical basis of biological reactions required for the propagation of genetic information stored in DNA and the organic chemistry principles behind the structure and function of nucleic acids.Main topics of lectures and class discussion will include the chemical and biochemical syntheses, properties and analyses of natural and modified nucleic acids to investigate cellular processes such as transcription, RNA splicing, other RNA regulation and translation; an introduction to the enzymatic strategies that accelerate these chemical reactions and a comparison of protein enzymes, ribozymes and other nucleic acid based enzymes in contemporary chemistry and biology. Students will learn to critically evaluate current scientific efforts that examine various aspects of chemistry and biological chemistry, the relationship between the structure and function of biomolecular systems, propose experiments to examine biological chemistry research problems and communicate these ideas and participate in scientific discussions and debates. 3 hrs. lec.

## 09-531 Polymer Science

### Fall: 9 units

Polymer science is a vibrant multidisciplinary activity. It uses the methods of chemistry, physics, chemical engineering, materials science and biology to create a coherent picture of the macromolecular world. This course is a survey of this field of endeavor suitable for Senior chemistry majors, or other students with a desire for a broad knowledge of the science and engineering of polymers. It covers a thorough description of the field, the synthetic chemistry of macromolecules, the physical chemistry of macromolecules, and the principles of polymer engineering and processing. Prerequisites: (09-219 or 09-217) and (09-214 or 09-345 or 09-347)

#### 09-534 Environmental Chemistry

## Spring: 9 units

Solar energy and electrical energy from renewable resources need to be stored to resolve intermittency issues. Energy can be stored through charge transfer, changes in chemical bonding, or in electric polarization. This course will introduce students to general aspects of energy-storage technologies using these strategies, integrating scientific and engineering perspectives to discuss thermodynamics, mechanisms of energy storage, and fundamental aspects of efficiency, capacity, and power delivery. Then we will explore current and experimental technologies, covering supercapacitors, batteries, and water-splitting catalysts. By the end of the course, students will be able to apply chemical principles to understand energy-storage technologies and gain knowledge of important classes of these systems. Students enrolled in 09-734 (rather than 09-534) will also be required to write a 15-page NSF style proposal. 3 hrs. lec. Prerequisites: (09-217 or 09-219) and (09-345 or 09-347 or 24-324 or 27-215 or 33-341)

## 09-535 Applied topics in Macromolecular and Biophysical Techniques

#### Fall: 9 units

Applications of physical chemistry are widespread. Physical chemical principles are fundamental to the methods used to sequence human genome, obtain high resolution structures of proteins and complex nucleic acids e.g., ribosome, and further provides the framework to predict how molecules fold in 3-dimension, how the different domains interact (inter- and intra-molecular interactions) to perform biological functions. The principles that were discussed in theory in undergraduate physical chemistry classes, will be applied in order to understand the molecular structures and dynamics in nucleic acids and proteins, and to more advanced molecular motors. In the last decade major advances have been made through single-molecule studies that provide finer details of macromolecules in action. This course aims to teach and apply physical chemistry as related to biological problems. Prerequisites: (09-345 or 09-214 or 09-347) and (03-121 or 03-231 or 03-232)

## 09-538 Exposure and Risk Assessment for Environmental Pollutants

#### All Semesters: 9 units

Our world is full of synthetic and naturally occurring toxic chemicals, presenting an imminent but difficult-to-quantify threat for human and ecosystem health. In this papers-based course we will ask the question, "How do we decide what's 'safe'?" in the context of exposure and risk assessment for toxic environmental pollutants. We will complete a series of case studies featuring current and seminal literature, in-class activities, and project-based assignments. Each case study will focus on a distinct contaminant exposure scenario and will be linked back to the common theme of using chemistry to understand how external exposure leads to internal dose and subsequent health impacts for diverse environmental pollutants. We will discuss how knowledge generated in the laboratory can be translated and used to inform regulatory decisions. The first half of the course will focus on contaminant bioavailability, exposure, and toxic effects in aquatic organisms. In the second half of the course, we will discuss human exposure to toxic pollutants and strategies to assess risks in the human population, including the human exposime concept, -omics-based research, and strategies for discovering novel harmful contaminants. Prerequisites: 09-105 or 09-107 or 09-106

### 09-560 Computational Chemistry

#### Fall: 12 units

Computer modeling is playing an increasingly important role in chemical, biological and materials research. This course provides an overview of computational chemistry techniques including molecular mechanics, molecular dynamics, electronic structure theory and continuum medium approaches. Sufficient theoretical background is provided for students to understand the uses and limitations of each technique. An integral part of the course is hands on experience with state-of-the-art computational chemistry tools running on graphics workstations. This course I can count towards coursework requirements for chemistry PhD candidates. 3 hrs. lec. Prerequisites: 09-347 or 09-345 or 09-344 or 09-214

#### 09-561 Computational Chemistry

#### Spring: 9 units

Computer modeling is playing an increasingly important role in chemical, biological and materials research. This course provides an overview of computational chemistry techniques including molecular mechanics, molecular dynamics, electronic structure theory and continuum medium approaches. Sufficient theoretical background is provided for students to understand the uses and limitations of each technique. An integral part of the course is hands on experience with state-of-the-art computational chemistry tools running on graphics workstations. This course I can count towards coursework requirements for chemistry PhD candidates. 3 hrs. lec.

## 09-563 Molecular Modeling and Computational Chemistry

#### Spring: 9 units

Computer modeling is playing an increasingly important role in chemical, biological and materials research. This course provides an overview of computational chemistry techniques including molecular mechanics, molecular dynamics, electronic structure theory and continuum medium approaches. Sufficient theoretical background is provided for students to understand the uses and limitations of each technique. An integral part of the course is hands on experience with state-of-the-art computational chemistry tools running on graphics workstations. This course I can count towards coursework requirements for chemistry PhD candidates. 3 hrs. lec. Prerequisites: 09-347 or 09-344 or 09-214 or 09-345

## **09-604 Introduction to Chemical Kinetics**

#### Spring: 6 units

Empirical description of the time evolution of chemical reactions. Inductive derivation of kinetic rate laws from actual data. Deductive derivation of kinetic rate laws from proposed mechanisms. Gas phase reactions, catalyzed reactions, enzyme kinetics. Theories of kinetic rate constants for gas phase reactions: unimolecular and bimolecular. Theories of solution phase reactions. Absolute reactions rate theory. Diffusion controlled reactions. Kinetics in highly viscous media. Activation energy and entropy. Volume of activation.

## 09-611 Chemical Thermodynamics

#### Fall: 6 units

This course provides an introduction to the general formalism of macroscopic thermodynamics and its applications to chemical systems. The main topics to be covered include: entropy maximum postulate, internal energy minimum postulate, various equilibrium conditions including chemical equilibrium, Legendre transformation and free energies, thermochemistry, phase equilibria and solution systems. Prerequisites: 09-231 and 09-345

## 09-614 Spectroscopy

## Intermittent: 6 units

This is a course exclusively in optical methods, both time resolved and steady state. In addition to methodology, spectral interpretation in terms of group theory will be discussed. The time-dependent formalism of quantum mechanics will also be introduced. Molecules in gas phase and condensed phase will be discussed. Frequent use will be made of the current literature. Background consisting of undergraduate physical chemistry is assumed. This course has a prerequisite 09-344, Quantum Chemistry or permission of the instructor.

## 09-615 Computational Modeling, Statistical Analysis and Machine Learning in Science

#### Fall: 12 units

The purpose of this course is to provide a practical introduction to the core concepts and tools of machine learning in a manner easily understood and intuitive to STEM students. The course begins by covering fundamental concepts in ML, data science, and modern statistics such as the bias-variance tradeoff, overfitting, regularization, and generalization, before moving on to more advanced topics in both supervised and unsupervised learning. Students will choose a large dataset from a selection of biology, chemistry, math, or physics datasets hosted by PSC and use this dataset throughout the MS program. The topics of the course are taught with students analyzing the chosen dataset. An intensive knowledge of Python or another computing language is not a pre-prerequisite since students will be given at first simple scripts that they work with and then expand upon. This course is required for students enrolled in the MS program in Data Analytics for Science.

Prerequisites: (09-344 or 09-231) and (15-110 or 15-112)

## 09-616 Neural Networks & Deep Learning in Science

#### Spring: 12 units

Focus on practice and applications of deep learning by exploring foundational concepts, structuring popular networks and implementing models through modern technologies (python, Jupyter notebooks and PyTorch). Other topics may include image recognition, machine translation, natural language processing, parallelism, GPU distributed computing, cloud technologies, inference and parameter tting in deep networks. Course uses large datasets hosted by PSC.

#### 09-621 Welcome to the Future Lab - Science in the Cloud

## Fall: 6 units

You can be at home or anywhere in the world and still run experiments in a lab. This course is to introduce and train students in the use of an automated and remote cloud lab facility. Operations in the cloud lab are conducted through a computer console and internet access that allows the user to program equipment, set up experiments and analyze data. In this course, students will learn the steps to use the Wolfram language/ Mathematica based Cloud Lab Command Center interface to remotely interact with the facilities and laboratory instruments in the cloud lab. Following training exercises, students will be able to select the appropriate equipment and reagents to prepare samples and solutions for laboratory analyses and experiments. (No prior knowledge of Mathematica is required but basic programming skills are helpful)

## 09-623 Future Lab- DNA Science in the Cloud

#### Fall: 6 units

This course uses an automated and remote cloud lab facility and will involve learning the steps to handle, manipulate and quantitate solutions of DNA and nucleic acids. Students will set up experiments that automate the dispensing, analysis and purification of nucleic acids and use DNA for biophysical measurements. Students will learn to remotely operate, design and execute experiments on state-of-the-art instrumentation to analyze DNA sequence and structure. Besides learning how to remotely use equipment and instruments for synthesis and analyses by spectroscopy and spectrometry, students will also learn about nucleic acids as part of their experiments. (Prior training in the use of the cloud lab is required) Prerequisite: 09-621 Min. grade C

## 09-701 Quantum Chemistry I

## Fall: 12 units

The main topics to be covered will include exploration of the Schroedinger equation, operators, particle in the box, harmonic oscillator and hydrogen atom, tunneling, Stern-Gerlach experiment and quantum mechanical postulates, time-independent and time-dependent perturbation theory, matrix diagonalization. The student will learn to master the fundamental concepts and techniques of quantum mechanics. The parallel mini course Mathematical Analysis for Chemistry will provide the necessary mathematical background.

## 09-702 Statistical Mechanics and Dynamics

## Intermittent: 12 units

This course will address the application of statistical mechanics to chemical systems. Topics to be discussed include the calculation of thermodynamic functions, phase transitions and chemical equilibrium, calculation of the transport properties of gases and liquids and the elementary theory of chemical kinetics.

Prerequisites: (09-611 or 09-344) and 09-231 and 09-701

## 09-705 Chemosensors and Biosensors

#### Intermittent: 12 units

Chemosensors and biosensors rely on "recognition" and "signaling" elements to transduce a molecular-scale binding event into an observable signal. Students in this course will be introduced to current research and technology for detecting chemical and biological analytes in a variety of contexts, including environmental testing, biological probing and medical diagnostics. Recognition elements ranging from small organic molecules to antibodies will be presented, while various detection modes, including fluorescence, gravimetric and colorimetric, that illustrate different signaling elements will be discussed and compared. Issues to be addressed include sensitivity, selectivity and efficiency. Each sensor will be analyzed in terms of the physical chemistry, organic chemistry and/or biochemistry underlying its function. This is a graduate level course that may also be appropriate for upper level undergraduates in chemistry and the biological sciences. The material in 09-518/09-519 or 09-718/09-719 would be appropriate background material for this course. 3 hrs. lec.

Prerequisites: (03-121 or 03-232 or 03-231) and (09-220 or 09-218)

## 09-707 Nanoparticles

#### Intermittent: 12 units

This course discusses the chemistry, physics, and biology aspects of several major types of nanoparticles, including metal, semiconductor, magnetic, carbon, and polymer nanostructures. For each type of nanoparticles, we select pedagogical examples (e.g. Au, Ag, CdSe, etc.) and introduce their synthetic methods, physical and chemical properties, self assembly, and various applications. Apart from the nanoparticle materials, other topics to be briefly covered include microscopy and spectroscopy techniques for nanoparticle characterization, and nanolithography techniques for fabricating nano-arrays. The course is primarily descriptive with a focus on understanding major concepts (such as plasmon, exciton, polaron, etc.). The lectures are power point presentation style with sufficient graphical materials to aid students to better understand the course materials. Overall, this course is intended to provide an introduction to the new frontiers of nanoscience and nanotechnology. Students will gain an understanding of the important concepts and research themes of nanoscience and nanotechnology, and develop their abilities to pursue highly disciplinary nanoscience research. 3 hrs. lec.

## 09-710 Chemistry and Sustainability

### Spring: 12 units

This course aims to educate students in the foundations of systematic leadership through chemistry and more for building a sustainable world. Many sustainability challenges are associated with commercial chemicals and with operational modes of the chemical enterprise. The course aims to challenge students to analyze and understand the root causes of unsustainability, especially in the technological dimension, to imagine a more sustainable world and to begin to define personal leadership missions. Students will be introduced to sustainability ethics as the foundation of transformative sustainability leadership, to a sustainability compass, to a Code of Sustainability Ethics and to various other helpful conceptual material as tools for analyzing the reasons our civilization has been failing to address its own unsustainability. The Collins Bookcase of Green Science Challenges organizes the technical content. It systematizes the major chemical sustainability challenges of our time: clean synthesis, renewable feed-stocks, safe energy, elemental pollutants, persistent molecular toxicants and endocrine disrupting chemicals (EDCs). Focal areas will be the technical, toxicological and cultural histories of elemental and molecular pollutants with particular emphasis on EDCs. Students will experience Legacy Lectures from some of the world's leading endocrine disruption scientists. The graded substance will take the form of take-home work. Students will primarily watch classic movies and read key books and articles and will summarize and personally evaluate the material in essay assignments. The course is intended for upper-level undergraduates and graduates although it is open to all students. The class is limited to 30 students. The assignments are common to both undergraduate and graduate classes offerings and 09-710 students will engage in additional projects. 3 hrs. lec.

Prerequisites: 09-107 or 09-105

## 09-711 Physical Organic Chemistry

## Fall: 12 units

This course introduces students to the study of structure and reactivity of organic compounds from a physical and theoretical standpoint. Students will learn the fundamentals of molecular orbital theory along with some practical applications to aromaticity and anti-aromaticity. Methods are described for the study of reaction mechanisms by means of physical methods such as kinetics, isotope effects, substituent effects, and solvent effects. Important reactive intermediates are described, along with detection methods. This course may be suitable for upper level undergraduates in chemistry with the appropriate background in organic chemistry and physical chemistry. 3 hrs. lec.

Prerequisites: (09-220 or 09-218) and (09-347 or 09-344)

#### 09-714 Advanced Organic Chemistry

#### Spring: 12 units

This course will expose the students to modern methods of organic synthesis including insights into the basis and mechanisms of chemical reactions. Topics include but are not limited to: modern spectroscopic analysis and structure determination, synthetic methods, retrosynthesis, organic reaction mechanisms, and references to separation techniques and some analytical methods. Upon completion of the course students should be able to design reaction schemes using scientific literature sources, evaluate their suitability for use in the lab and develop an aptitude in identifying the use of modern reagents that are more efficient, specific, safer and environmentally friendly. It is assumed that at minimum students will have completed at least two semesters of undergraduate coursework in organic chemistry and suggested that they have completed 09-222 and 09-321, the organic laboratory courses. 3 hrs. lec Prerequisites: 09-220 or 09-218

09-715 Physical Chemistry of Macromolecules

## All Semesters: 12 units

This course addresses the fundamentals of polymer science with the emphasis on physicochemical consequences of chain nature of macromolecules and on the behavior of polymers in condensed state (polymers as soft condense matter). The topics to be covered include: chain structure and molecular weight; molecular weight distribution; step growth and addition polymerization mechanisms; chain conformation and behavior of polymers in solution; concentrated solutions and phase separation behavior; rubber elasticity; introduction to polymer viscoelasticity and rheology; mechanical behavior of polymers; glass transition and crystallization; multicomponent polymeric materials; liquid crystalline polymers; polymers at surfaces and interfaces; self-assembly and nanostructure formation in synthetic and biological systems; conducting and semiconducting polymers. Graduate students taking the course for 12 units will be required to write a term paper on a selected topic. 3 hrs. lec. Prerequisites: 06-310 or 09-345

#### **09-716 Bioactive Natural Products**

## Spring: 12 units

This course is aimed at students with an interest in natural products research. Natural products are used as active components in medicinal products, as model compounds for further development into medicinally active drugs, as ingredients in food and for flavor and fragrances, among other very useful and interesting applications. An overview of the structural variety and activity of natural products will be presented along with their isolation and structural determination. Overall, the course will offer an introduction to the work that is customary in natural product research. This course will cover: Strategies to select the plant or marine material for study; main groups of natural products derived from plants; representative natural products derived from marine organisms; preparation of extracts and selection of active fractions, screening strategies; separation and purification of active components; bench-top bioassays and chemical assays and structure elucidation (especially 2D-NMR spectroscopy) Student's performance will be assessed by weekly assignments on the topics discussed in lecture and exams. 3 hrs. lec. Prerequisites: 09-219 or 09-217

## 09-718 Bioorganic Chemistry: Nucleic Acids and Carbohydrates

## Fall: 12 units

This course will introduce students to new developments in chemistry and biology, with emphasis on the synthesis, structural and functional aspects of nucleic acids and carbohydrates, and their applications in chemistry, biology and medicine. Later in the course, students will have the opportunity to explore cutting-edge research in this exciting new field that bridges chemistry with biology. Students will be required to keep abreast of the current literature. In addition to standard homework assignments and examinations, students will have the opportunity to work in teams to tackle contemporary problems at the forefront of chemistry and biology. The difference between the 09-518 (9-unit) and 09-718 (12-unit) is that this latter is a graduate level course. Students signed up for 09-718 will be required to turn in an original research proposal at the end of the course, in addition to all the other assignments. 3 hrs. lec. Prerequisites: (03-121 or 03-151) and (09-220 or 09-218)

#### 09-719 Bioorganic Chemistry: Peptides, Proteins and Combinatorial Chemistry

Spring: 12 units

This course will introduce students to new developments in chemistry and biology, with emphasis on the synthesis, structural and functional aspects of peptides, proteins and small molecules. Basic concepts of bioorganic chemistry will be presented in the context of the current literature and students will have the opportunity to learn about the experimental methods used in various research labs. An introduction to combinatorial chemistry in the context of drug design and drug discovery will also be presented. Students will be required to keep abreast of the current literature. Homeworks and team projects will be assigned on a regular basis. The homework assignments will require data interpretation and experimental design; and team projects will give students the opportunity to work in teams to tackle contemporary problems at the interface of chemistry and biology. Students enrolled in the graduate level course (09-719) will be required to turn in an original research proposal at the end of the course, in addition to the homework assignments, midterm, and final exam that are required for the undergraduate course. Prerequisites: (03-121 or 03-151) and (09-218 or 09-220)

#### 09-720 Physical Inorganic Chemistry

Intermittent: 6 units

This course develops the principles of magnetochemistry and inorganic spectroscopy. Electronic absorption, magnetic circular dichroism, resonance raman, NMR, EPR, Mossbauer, magnetization and x-ray methods will be introduced with application towards the determination of electronic structures of transition metal complexes. Prerequisites: 09-344 and 09-348 and 09-345

## 09-721 Metals in Biology: Function and Reactivity

#### Intermittent: 6 units

Metal ions play important roles in many biological processes, including photosynthesis, respiration, global nitrogen cycle, carbon cycle, antibiotics biosynthesis, gene regulation, bio-signal sensing, and DNA/RNA repair, just to name a few. Usually, metal ions are embedded in protein scaffold to form active centers of proteins in order to catalyze a broad array of chemical transformations, which are essential in supporting the biological processes mentioned above. These metal containing proteins, or metalloproteins, account for half of all proteins discovered so far. In this course, the relation between the chemical reactivity and the structure of metalloproteins will be discussed in detail. The main focus is to illustrate the geometric and electronic structure of metal centers and their interactions with the protein environment in governing the chemical reactivity of metalloproteins. The applications of these principles in designing biomimetic/bioinspried inorganic catalysts and in engineering metalloproteins bearing novel chemical reactivity will also be discussed. The basic principles of the frequently utilized physical methods in this research area will also be introduced, which include optical absorption spectroscopy, Infrared (IR) and Raman spectroscopies, M and #246;ssbauer spectroscopy, electron paramagnetic resonance (EPR), X-ray absorption and diffraction techniques. Prerequisites: (09-344 or 09-214 or 09-347 or 09-345) and 09-348

## 09-722 Kinetics and Mechanisms of Chemical and Enzymatic Reactions

#### Intermittent: 12 units

This is a practical course aimed at learning the major modern tools which are essential for investigation of mechanisms of homogeneous chemical and enzymatic reactions. Rules of formal chemical kinetics in solution are first considered followed by basic principles of kinetics of enzymatic processes including inhibition, which is a key factor in the up-to-date drug design. The relationships between electronic structures, catalytic properties, and reactivity of biologically relevant metal complexes will be provided. Electrochemical and redox features of metal complexes will be reviewed. The course includes such hot topics as Fenton chemistry, Marcus's electron transfer concept, catalysis by Collins' TAML activators of peroxides, specific and general acid/base, proximal and micellar catalysis. Mechanistic pathways of action of hydrolases, kinases, hydrogenases, oxidases, peroxidases, cytochrome P-450, and other metalloenzymes will be described. The course is supplied by the recently published text (A. D. Ryabov "Practical Kinetics and Mechanisms of Chemical and Enzymatic Reactions" Cambridge Scholars Publishing, Newcastle upon Tyne, NE6 2PA, UK) which includes all the above mentioned themes (Graduate course: 09-722, 12-units) 3 hrs. lec. Prerequisite: 09-348 Prerequisites: 09-345 and 09-220 and 09-348

## 09-723 Proximal Probe Techniques: New Tools for Nanoscience & Nanotechnology

#### Intermittent: 12 units

Proximal probe techniques are revolutionizing physical and biological sciences, owing to their ability to explore and manipulate matter at the nanoscale, and to operate in various environments (including liquids). Proximal probe techniques rely on the use of nanoscale probes, positioned and scanned in the immediate vicinity of the material surface. Their development is often viewed as a first step towards nanotechnology, since they demonstrate the feasibility of building purposeful structures one atom or one (macro)molecule at a time. This course is designed for the students of chemistry, biology physics and engineering, who are interested in the fundamentals of proximal probe techniques and in their applications in various areas, converging into a rapidly developing, interdisciplinary field of nanoscience. It will provide physical background of such basic techniques as Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM), and Near-Field Scanning Optical Microscopy (NSOM) and of their variants. Throughout the course, the working "virtual AFM" computer model will be assembled in classroom by each student and then used extensively to gain thorough understanding of AFM operation principles. Particular emphasis will be placed on modes of operation facilitating chemical contrast and contrast based on other material properties. (No prior experience with computer programming required). 3 hrs. lec. Prerequisites: (21-124 or 21-122 or 09-231) and (09-344 or 09-331 or

Prerequisites: (21-124 or 21-122 or 09-231) and (09-344 or 09-331 or 09-322 or 09-345)

## 09-724 Environmental Chemistry

## Spring: 12 units

. Environmental pollutants are common consequences of human activities. These chemicals have a wide range of deleterious effects on the environment and people. This course will introduce students to a range of major environmental pollutants, with a particular focus on persistent organic pollutants. We will use chemical principles including thermodynamics, kinetics, photochemistry, organic reaction mechanisms, and structure activity relationships to understand the environmental fate of major classes of pollutants. The transport of chemicals through the environment and their partitioning between air, water, soil, and people will be described. The major environmental reaction pathways (oxidation, photolysis, hydrolysis, reduction, metabolism) of common pollutants will be explored. This will provide students with the necessary knowledge to predict the chemical fate of environmental pollutants, and improve their understanding of the service and a point and so that a service and a service and a service and a service. Specific topics include water quality, photochemical smog, organic aerosols, atmospheric chemistry and global climate change, toxicity of pesticides, and heterogeneous and multiphase atmospheric chemistry. This 12-unit course is intended for graduate students that want to explore aspects of the course more deeply. This includes additional requirements including a final term paper and in-class presentation, and additional advanced questions on the homework assignments. Undergraduates should register for 09-524, the 9unit version of the class, unless they obtain specific permission from the instructor to enroll in this class. Prerequisites: 09-217 or 09-219

## 09-729 Introduction to Sustainable Energy Science

## Fall: 12 units

This course focuses on the chemistry aspects of sustainable energy science. It introduces the major types of inorganic and molecular materials for various important processes of energy conversion and storage, such as photovoltaics, fuel cells, water splitting, solar fuels, batteries, and CO2 reduction. All the energy processes heavily rely on innovations in materials. This course is intended to offer perspectives on the materials/physical chemistry that are of importance in energy processes, in particular, how the atomic and electronic structures of materials impact the energy harvesting and conversion. In current energy research, intense efforts are focused on developing new strategies for achieving sustainable energy through renewable resources as opposed to the traditional oil/coal/gas compositions. This course offers students an introduction to the current energy research frontiers with a focus on solar energy conversion/ storage, electrocatalysis and artificial photosynthesis. The major types of materials to be covered include metals, semiconductors, two-dimensional materials, and hybrid perovskites, etc. The material functions in catalysis, solar cells, fuel cells, batteries, supercapacitors, hydrogen production and storage are also discussed in the course. The lectures are power-point presentation style with sufficient graphical materials to aid students to better understand the course materials. Demo experiments are designed to facilitate student learning

Prerequisites: (09-105 or 09-107) and (33-151 or 33-121 or 33-141)

## 09-730 Chemistry of Gene Expression

#### Fall: 12 units

rinciples behind the structure and function of nucleic acids.Main topics of lectures and class discussion will include the chemical and biochemical syntheses, properties and analyses of natural and modified nucleic acids to investigate cellular processes such as transcription, RNA splicing, other RNA regulation and translation; an introduction to the enzymatic strategies that accelerate these chemical reactions and a comparison of protein enzymes, ribozymes and other nucleic acid based enzymes in contemporary chemistry and biology. Students will learn to critically evaluate current scientific efforts that examine various aspects of chemistry and biological chemistry, the relationship between the structure and function of biomolecular systems, propose experiments to examine biological chemistry research problems and communicate these ideas and participate in scientific discussions and debates. 3 hrs. lec.

#### 09-732 Biocatalysis: Fundamentals, Recent Advances and Industrial Applications

#### Fall: 6 units

Biocatalysis is a rapidly developing field that utilizes naturally evolved and bioengineered enzymes as platforms to offer revolutionary solutions for chemical production. Modern biocatalysis relies on enzyme discovery, enzyme reaction mechanism elucidation, and high throughput screening processes for enzyme bioengineering. The recent established world's first academic cloud lab at CMU is a perfect remote-access and automated facility to be used to expand our research capacity into the biocatalysis area in both fundamental studies and biocatalytic platform development and engineering. This great research and educational opportunity calls for the development of courses to disseminate fundamental knowledge and practical skills related to biocatalysis to students so that the interested students could start engaging in this area of research. Thus, this proposed course, with the aim to introduce the field of biocatalysis in both academic studies and industrial applications, starts filling this gap. This course features an in-depth discussion of different topics in biocatalysis with examples of how biocatalysis has reshaped various aspects of modern industries including food, pharmaceuticals, consumer products and biomaterials industries. This course also provides an overview of common enzyme classes used in modern biocatalysis and their associated catalytic mechanisms and engineering. Hands-on experience of common bioinformatic and computational tools for new enzyme discovery will also be integrated into the course. Prerequisites: (09-219 or 09-217) and (03-231 or 03-151 or 03-121 or

Prerequisites: (09-219 or 09-217) and (03-231 or 03-151 or 03-121 or 03-232)

## 09-736 Transition Metal Catalysis for Organic and Polymer Synthesis

## Intermittent: 12 units

Transition metal catalysts are invaluable in small molecule and polymer synthesis. The course will begin with a brief overview of organometallic chemistry and a discussion of fundamental organometallic reactions. Following this, a survey of some selected topics for the formation of small molecules and polymers will be presented. Some topics to be highlighted include: (1) Hydrogenation (2) Palladium Catalyzed Cross-Coupling (3) Epoxidation (4) Olefin Metathesis (5) Olefin Polymerization Prerequisites: (09-218 or 09-220) and 09-348

### 09-737 Medicinal Chemistry and Drug Development

#### Spring: 12 units

Organic chemistry is an intimate part of the drug discovery and design processes in areas that include structure determination (NMR, mass spectrometry), synthesis, and determination of mechanisms of action. Once a promising compound (i.e. a ?lead?) has been identified in the laboratory, it is rarely ready to be used in the clinic. Complications include poor bioavailability, rapid degradation, and off-target effects. Students will learn about lead compound optimization through structural variations, cell-specific targeting and pro-drug strategies. Several examples will be presented to illustrate the role played by organic chemistry in the development of drugs used to treat a range of diseases, including cancer, HIV-AIDS, bacterial infections and heart disease. Prerequisites: 09-220 or 09-218

## 09-738 Exposure and Risk Assessment for Environmental Pollutants

#### Intermittent: 12 units

Our world is full of synthetic and naturally occurring toxic chemicals, presenting an imminent but difficult-to-quantify threat for human and ecosystem health. In this papers-based course we will ask the question, "How do we decide what's 'safe'?" in the context of exposure and risk assessment for toxic environmental pollutants. We will complete a series of case studies featuring current and seminal literature, in-class activities, and project-based assignments. Each case study will focus on a distinct contaminant exposure scenario and will be linked back to the common theme of using chemistry to understand how external exposure leads to internal dose and subsequent health impacts for diverse environmental pollutants. We will discuss how knowledge generated in the laboratory can be translated and used to inform regulatory decisions. The first half of the course will focus on contaminant bioavailability, exposure, and toxic effects in aquatic organisms. In the second half of the course, we will discuss human exposure to toxic pollutants and strategies to assess risks in the human population, including the human exposome concept, -omics-based research, and strategies for discovering novel harmful contaminants. Prerequisites: 09-107 or 09-106 or 09-105

## 09-741 Organic Chemistry of Polymers

## Spring: 12 units

A study of the synthesis and reactions of high polymers. Emphasis is on practical polymer preparation and on the fundamental kinetics and mechanisms of polymerization reactions. Topics include: relationship of synthesis and structure, step-growth polymerization, chain-growth polymerization via radical, ionic and coordination intermediates, copolymerization, discussions of specialty polymers and reactions of polymers. Students in 09-741 will take the same lectures and the same exams as those enrolled in 09-502 but, in addition, will prepare a term paper on the topic of advanced polymeric materials, to be approved by the instructor. 09-509 or 09-715, Physical Chemistry of Macromolecules, is excellent preparation for this course but is not required. 3-6 hrs. lec.

## 09-760 The Molecular Basis of Polymer Mechanics

## Spring: 12 units

This course is a graduate level course designed to prepare students for graduate research in polymer science. Based around a laboratory component, students will learn the lab skills needed to synthesize and fully characterize novel polymer materials. The classroom component will teach the theory behind the measurements made in lab, as well as an understanding of the best experiments to learn about the properties of the material. Emphasis will be placed on current literature and technical communication (written and oral). 3 hrs lec; 3 hrs lab

## 09-763 Molecular Modeling and Computational Chemistry

#### Spring: 12 units

Computer modeling is playing an increasingly important role in chemical, biological and materials research. This course provides an overview of computational chemistry techniques including molecular mechanics, molecular dynamics, electronic structure theory and continuum medium approaches. Sufficient theoretical background is provided for students to understand the uses and limitations of each technique. An integral part of the course is hands on experience with state-of-the-art computational chemistry tools running on graphics workstations. This is the graduate equivalent of 09-563. Students enrolled in the graduate level course will complete an additional independent project. 3 hrs. lec.

## 09-768 Machine Learning for Molecular Sciences

#### Spring: 12 units

The emergence of contemporary artificial intelligence (AI) and machine learning (ML) methods has the potential to substantially alter and enhance the role of computers in science. At the heart of ML applications, lie statistical algorithms whose performance, much like that of a scholar, improves with training. There is a growing infrastructure of machine learning tools for generating, testing and refining scientific models. Such techniques are suitable for addressing complex problems that involve vast combinatorial spaces or complex processes, which conventional procedures either cannot solve or can tackle only at great computational cost. The purpose of this course is to provide a practical introduction to the core concepts and tools of machine learning in a manner easily understood and intuitive to STEM students. The course begins by covering fundamental concepts in ML, data science, and modern statistics such as the biasvariance tradeoff, overfitting, regularization, and generalization, before moving on to more advanced topics in both supervised and unsupervised learning. Topics covered in the course also include ensemble models. neural networks, modern deep learning, embedding, clustering and data visualization. Throughout the course, we emphasize application of ML methods to chemical, physical and biological data. A notable aspect of the course is the hands-on use of Python Jupyter notebooks to introduce modern ML/statistical packages.

Prerequisites: (09-344 or 09-231) and (15-112 or 15-110)

## 09-803 Chemistry of Gene Expression

#### Intermittent: 12 units

This course examines the chemical basis of biological reactions required for the propagation of genetic information stored in DNA and the organic chemistry principles behind the structure and function of nucleic acids.Main topics of lectures and class discussion will include the chemical and biochemical syntheses, properties and analyses of natural and modified nucleic acids to investigate cellular processes such as transcription, RNA splicing, other RNA regulation and translation; an introduction to the enzymatic strategies that accelerate these chemical reactions and a comparison of protein enzymes, ribozymes and other nucleic acid based enzymes in contemporary chemistry and biology. Students will learn to critically evaluate current scientific efforts that examine various aspects of chemistry and biological chemistry, the relationship between the structure and function of biomolecular systems, propose experiments to examine biological chemistry research problems and communicate these ideas and participate in scientific discussions and debates. 3 hrs. lec. Prerequisites: (09-218 or 09-220) and (03-231 or 03-232)