Chemistry

Contact:	Barbara Tessmer
Phone:	314-935-7316
Email:	barbara22@wustl.edu
Website:	http://www.chemistry.wustl.edu/graduate

Courses

CHEM 5000 Independent Work
Independent mentored work in Chemistry, such as (but not limited to) a detailed literature search and report on a topic of current interest.
Credit 0.5-6 units.
Typical periods offered: Fall, Spring

CHEM 5001 Physical Science in 12 Problems
Exercises related to general chemistry, classical mechanics, quantum mechanics, statistical mechanics, thermodynamics, and kinetics, will be solved with numerical software. Each exercise will be accompanied by a lecture, a software template solving a problem and presenting a related take-home problem. The software will allow us to focus on, and treat in a transparent fashion, physical problems without the unworldly idealizations and contrivances found in textbooks. Prerequisites: Chem 106/112A and/or Physics 192/194, and prior or concurrent enrollment in either Chem 401 or Phys 217. The lectures will be in-person however a complete set of taped lectures will also be available. A remote help session will be scheduled at a mutually agreed to time. There are no quizzes, exams or a final.
Credit 1 unit. A&S IQ: NSM Art: NSM

CHEM 5010 Physical Chemistry I
Introduction to quantum chemistry with applications to electronic structure and elementary spectroscopy.
Credit 3 units. A&S IQ: NSM Art: NSM BU: SCI
Typical periods offered: Fall

CHEM 5011 Quantum Chemistry and Spectra
This course covers the development and application of quantum mechanics as applied to molecular structure and properties. Material to be discussed will include the fundamentals of quantum mechanics; representations; matrix formalisms; applications to model systems; perturbation theory; variational methods; many-electron wavefunctions; Hartree-Fock theory and post-Hartree Fock methods; density functional theory; additional topics and applications. Prereq: Chem 401.
Credit 3 units.
Typical periods offered: Fall

CHEM 5012 Advanced Quantum Chemistry
A study of the theory and methods of quantum mechanics, with applications to problems of chemical interest. Prerequisite, Chem 571 or permission of the instructor.
Credit 3 units.

CHEM 5014 Physical Properties of Quantum Nanostructures
This course will explore the physical properties of semiconductor nanomaterials with dimensions that are small enough to give rise to quantum-confinement effects. These effects strongly influence the electronic structures, absorption/emission behavior, and charge-carrier dynamics within quantum wells, rods, wires, dots, and nanotubes. The course begins with an overview of the electronic structure of bulk semiconductors. The theoretical and experimental bases for quantum-confinement effects, which are of considerable fundamental and applied interest, will then be developed. A significant emphasis will be placed on the optical absorption and photoluminescence properties of semiconductor quantum nanostructures. Recent advances and observations as reported in the literature will be emphasized throughout the semester. Prerequisites: Chem 461/Chem 5610 and Chem 465/Chem 5620, or permission of the instructor. While the course is steered to graduate students in the Chemistry Department, Chemistry undergraduate students, graduate or undergraduate students in Physics, Electrical & Systems Engineering, Energy, Environmental & Chemical Engineering, Mechanical Engineering & Materials Science may also find this course valuable.
Credit 3 units.
Typical periods offered: Spring

CHEM 5020 Physical Chemistry II
This course presents an introduction to chemical thermodynamics, statistical mechanics, and transport phenomena.
Credit 3 units. A&S IQ: NSM Art: NSM BU: SCI
Typical periods offered: Spring

CHEM 5021 Statistical Thermodynamics
Statistical mechanical methods will be used to characterize equilibrium and non-equilibrium thermodynamic systems. Computer programming assignments are given. An initial familiarity with ideal equilibrium systems will be assumed. Prerequisite Chem 401 or its equivalent or permission of the instructor.
Credit 3 units.

CHEM 5030 Chemical Kinetics
This lecture course will provide an introduction to the kinetics of chemical reactions for graduate and upper-level undergraduate science and engineering students. Bulk and molecular-level considerations will be discussed and provide a foundation for the understanding of chemical reaction mechanisms and the techniques used for their study. Students will gain an understanding of the importance and significance of the rate laws of reactions and in particular the reaction rate constant. Details of how the environment in which reactions occur (i.e., gas phase, solution phase, and surface reactions) and molecular structure are reflected in the rate constant will be discussed. Examples such as catalytic loss cycles in the atmosphere, enzyme catalysis, combustion systems, chain reactions, and explosions are presented in detail to illustrate how the fundamental principles of chemical kinetics can be applied to predict reaction rates, chemical reactivity, and the outcomes of particular processes. Prerequisites: Chem 106/112A and/or permission of instructor.
Credit 3 units. A&S IQ: NSM Art: NSM

CHEM 5031 Molecular Reaction Dynamics
This course addresses the question, what happens in a chemical reaction? at the atomic/molecular level. Topics: Non-reactive and reactive molecular collisions, scattering and resonances, unimolecular and bimolecular reactions, potential energy surfaces, reaction rate calculations and models, state to state experiments and stereodynamics, energy transfer mechanisms, time resolved and frequency resolved dynamics, condensed phase dynamics, control of chemical reactions. Requirements: Chem 401 is a pre-requisite and prior completion or current registration in Chem 402 is required. However, equivalent courses will be considered at the discretion of the instructor.
Credit 3 units.

CHEM 5035 Nuclear and Radiochemistry Lab
Application of radiochemistry to problems in chemistry, physics, and nuclear medicine, with emphasis on particle detectors and experimental techniques. Prerequisites: 3 units of physical chemistry or quantum mechanics, or permission of instructor. Five hours of laboratory a week.
Credit 3 units. A&S IQ: NSM Art: NSM
Typical periods offered: Fall

CHEM 5036 Introduction to the Atomic Nucleus
Introduction to the interaction of radiation with matter, the production and decay of radioactive nuclides, the structure and properties of nuclei, and various applications of nuclear science (including nuclear power) are all presented. Lectures will be in-person but a complete set of taped lectures will also be available. A weekly, in-person or remote, help session will be scheduled at a mutually agreed to time. There will be about 6 timed quizzes, one midterm and one final, all of which must be taken in-person on mutually agreed dates.
Credit 3 units. A&S IQ: NSM Art: NSM
Typical periods offered: Fall

CHEM 5041 Molecular Spectroscopy
Cursory overview of electromagnetic radiation and its interaction with atoms and molecules. The course will assume a general knowledge of quantum chemistry, (i.e., Chem 401), although a quick review of eigenfunctions and states will be given. We will cover Rotational Spectroscopy, Vibrational Spectroscopy, Electronic Spectroscopy, and Time-resolved Spectroscopy. In so doing, attention will be focused on diatomic molecules, although some examples of polyatomics will be given with emphasis placed on how structure contrbutes to spectra. Emphasis is placed on creating intuition into spectroscopy, not necessarily the quantum-mechanical rigor or detailed calculations of molecular spectroscopy. Prequisite, Chem 401 or permission of the instructor.
Credit 3 units.
Typical periods offered: Fall, Spring

CHEM 5042 Time-Dependent Quantum Mechanics & Spectroscopy
This graduate-level course lays the foundations of time-dependent quantum mechanics and applications to contemporary optical spectroscopies, particularly ultrafast techniques. Formal theoretical descriptions for nonlinear spectroscopic techniques including transient absorption, photon echo, and two-dimensional spectroscopies will be developed. Practical aspects of these experiments including modern laser systems, instrument design, data collection, data processing, and data analysis will also be discussed. Discussion of current literature in the field will be an important component of the course. Prerequisite courses: Chem 401 or permission from the instructor.
Credit 3 units.

CHEM 5050 Computational Problem Solving in the Chemical Sciences
Have you ever wondered how molecular interactions shape the world around us? Why do certain materials exhibit unique properties? How can we predict and manipulate chemical reactions at the atomic level? These are the mysteries at the heart of chemistry, where understanding the unseen world of atoms and molecules can unlock groundbreaking advances in science and technology. However, one needs specialized numerical methods and computational chemistry skills to explore these questions. This course is designed to bridge this gap. It provides a comprehensive introduction to the mathematical and computational skills necessary to model chemical phenomena at the atomic level. We start by building a strong foundation in mathematical representations of chemical problems, utilizing open-source software tools for problem-solving, data interpretation, and visualization of materials and molecular structures. In the second part of the course, we delve into the fascinating world of atomic-level computer modeling. You'll learn various methodologies, such as Monte Carlo and molecular dynamics. We'll analyze static (thermodynamic and structural) and dynamic properties and their statistical errors. Don't worry if you're new to coding - we'll cover the basics of Python programming in the first few lectures, setting you up for success. By the end of this course, you will be proficient in using computational tools, understanding atomic interactions, and approaching chemical problems with a structured and strategic thought process. Join us to unlock the secrets of the molecular world and transform the way you see chemistry! Prerequisites: Chem 106/112A, Math 132, Physics 191, Chem 261.
Credit 3 units. A&S IQ: NSM
Typical periods offered: Fall

CHEM 5051 Methods of Biophysical Chemistry
The course provides an overview of key methodologies of contemporary biophysics and biophysical chemistry, covering: 1) Spectroscopic methods routinely used in biochemistry, including absorption, fluorescence, and circular dichroism; 2) Biophysical methods to study intra- and intermolecular protein interactions including solutionstate NMR, FCS, and FRET; 3) Cutting-edge biophysical techniques to study transient proteinprotein/ protein-nucleic acids interactions. A significant emphasis is placed on the principles of quantum mechanics, which underpin all the techniques discussed. The course begins with an introduction to the basics of quantum mechanics, laying a foundation for understanding the core physical principles that govern each method. Throughout the course, we will derive and analyze key formulae essential for comprehending and applying these advanced biophysical techniques effectively.
Credit 3 units.
Typical periods offered: Fall

CHEM 5061 Magnetic Resonance
Quantum mechanical and classical aspects of paramagnetism and of nuclear and electronic magnetic resonance. Phenomenological equations of motion, spin intractions, spin temperature, thermal relaxation, dynamic polarization, multiple resonance phenomena.
Credit 3 units.
Typical periods offered: Spring

CHEM 5062 Special Topics in Physical Chemistry:
A course dealing with the quantum and classical description of the nuclear magnetic resonance of an isolated system of two spin-1/2 nuclei. The design of pulsed NMR spectrometers and the Fourier analysis of time-dependent observable magnetization in 1 and 2 dimensions are treated in detail, NMR relaxation in liquids and solids is included phenomenologically. Prerequisite: Physical Chemistry or permission of the instructor.
Credit 3 units.

CHEM 5063 Electron Spin Resonance
Principles of magnetic resonance of paramagnetic species, structure and dynamics of organic free radicals and transition metal ions in the condensed phase. Detection of transient paramagnetic species generated in photochemical reactions and photo physical processes. Prereq, Chem 401.
Credit 3 units.

CHEM 5064 NMR for Biological Solids
The course will cover theoretical and practical aspects of nuclear magnetic resonance (NMR) spectroscopy. Specific focus will be given to solid-state NMR and its application for studying amorphous biological solids. Prerequisites: undergraduate-level course in quantum mechanics.

Credit 3 units.

Typical periods offered: Fall

CHEM 5070 Instrumental Methods: Physical Chemistry

A course providing direct hands-on experience with the principles of physical chemistry (thermodynamics, quantum, kinetics) and associated experimental methods and instrumentation, including optical, infrared, and nuclear and electron spin resonance, electrochemistry, calorimetry, laser kinetics, and basic electronics. Prerequisite: Chem 401 or concurrent enrollment in Chem 402.

Credit 3 units. A&S IQ: NSM, WI Art: NSM

CHEM 5080 Special Topics in Physical Chemistry

This course will present a detailed focus on a particular topic of current interest in Physical Chemistry

Credit 3 units.

Typical periods offered: Fall

CHEM 5100 Chemical Laboratory Safety

An overview of current laboratory safety, regulatory, and compliance practices. Safety and compliance issues that impact chemical, biological, and materials research will be covered. Required for entering chemistry graduate students.

Credit 0.5 units.

Typical periods offered: Fall

CHEM 5101 Introduction to Online Chemical Information Sources

Intro to online searching of Chemical Abstracts database. Topics include assessing the benefits and limitations of online searching, developing and conducting effective and efficient bibliographic search, as well as learning the tools for building and searching chemical structures online.

Credit 0.5 units.

CHEM 5110 Thriving in Graduate School

This course will provide graduate students with a foundation of research, communication, and professional skills, with a focus on starting their thesis research project and preparing for second-year Chemistry program milestones. Students will work individually and in groups to refine their project ideas, make a plan for project implementation, communicate both in writing and orally to multiple audiences, and learn to navigate professional interactions such as networking, negotiation, and feedback. This course is intended to be taken in the first year of the graduate program.

Credit 3 units.

Typical periods offered: Spring

CHEM 5330 Time-Dependent Quantum Mechanics & Spectroscopy

This graduate-level course lays the foundations of time-dependent quantum mechanics and applications to contemporary optical spectroscopies, particularly ultrafast techniques. Formal theoretical descriptions for nonlinear spectroscopic techniques including transient absorption, photon echo, and two-dimensional spectroscopies will be developed. Practical aspects of these experiments including modern laser systems, instrument design, data collection, data processing, and data analysis will also be discussed. Discussion of current literature in the field will be an important component of the course. Prerequisite courses: Chem 401 or permission from the instructor.

Credit 3 units.

Typical periods offered: Fall, Spring

CHEM 5361 Radiochemistry for the Life Sciences

This course will provide an introduction to nuclear science (e.g. radioactive decay, nuclear stability, interactions of radiation with matter) and followed by an overview of how radiochemistry is used in the life sciences. Lectures on radiolabeling chemistry with radionuclides used in medical imaging (single photon emission computed tomography (SPECT) and positron emission tomography (PET) and their applications will be presented. In addition, lectures on radiochemistry with tritium (H-3) and C-14 will also be included. Additional applications include environmental radiochemistry as applied to nuclear waste disposal and biofuels.

Credit 2 units.

CHEM 5510 Organic Chemistry III

A lecture course that builds on the material in the first two semesters of Organic Chemistry, covering in more detail certain topics in those courses while also introducing new topics. A transition to graduate-level study in organic chemistry; recommended for chemistry, biochemistry, and biology majors.

Credit 3 units. A&S IQ: NSM Art: NSM

Typical periods offered: Fall

CHEM 5511 Synthetic Polymer Chemistry

This course that describes various methods for the synthesis and characterization of polymers. Copolymers, control of architecture, polymer reactivity, polymer properties, structure/property relationships, and applications of polymers will be discussed. Current topics of interest from the recent literature will also be covered. Prerequisite: Chem 262 or permission of instructor.

Credit 3 units. A&S IQ: NSM Art: NSM

CHEM 5512 Synthetic Methods

A lecture course presenting a detailed survey of synthetically useful reactions of carbonyl compounds and their derivatives, with particular attention to their stereoselectivity aspects and asymmetric methodology. The course is intended to provide the necessary background for more advanced work in organic synthesis.

Credit 3 units.

Typical periods offered: Spring

CHEM 5513 Advanced Organic Synthesis

The objective of this course is to teach students the art of planning a total synthesis. Key synthetic concepts, strategies and tactics, as well as a variety of reactions and synthetic methods, will be illustrated using examples from total syntheses of the main groups of natural products - terpenes, steroids, and alkaloids. Prerequisite: Chem 451/Chem 5510 or permission of instructor.

Credit 3 units.

Typical periods offered: Spring

CHEM 5521 Physical Organic Chemistry

The goal of physical organic chemistry (formerly called mechanistic organic chemisry) is to understand the details of reaction mechanisms, and gain insight into structures and reactivity common to organic chemicals and of high-energy chemical intermediates. This course focuses on the structure of any intermediates, the extent of a reaction from the perspective of the transition state, and identifying the relative energies of reactants, products, intermediates, and transition states. Students will learn concepts needed to solve mechanistic organic problems encountered in research, covering common organic reaction mechanisms, experimental techniques, and theoretical approaches.

After the course, students will be able to design experiments to probe mechanistic questions and propose reasonable mechanisms and intermediates to explain experimental observations. Prerequisite CHEM 262 or permission of the instructor.
Credit 3 units. A&S IQ: NSM Art: NSM BU: SCI

CHEM 5540 Molecular Orbital Theory
Lectures will cover the background, practice and applications of computational chemistry to the modeling of the structures and chemical reactions of organic molecules. Different levels of calculation will be presented, from molecular mechanics calculations and Hhckel molecular orbital theory, through semi-empirical and ab initio self-consistent field calculations with correlation energy corrections, and density functional theory. Hands-on experience performing calculations is an important element in this course.
Credit 3 units.

CHEM 5570 Synthetic Polymer Chemistry Laboratory
An upper-level laboratory course that complements Chem 5511 Synthetic Polymer Chemistry. This twice-a-week lab provides hands-on training in the design, synthesis, and characterization of polymers and polymeric materials through four standard experiments (each one week) and one independent project (over five to six weeks). The independent project involves using an article from the literature as the basis for developing a short proposal. At the end of the course, students give oral presentations of their proposals, which are reviewed by their classmates.
Credit 3 units. A&S IQ: NSM Art: NSM BU: SCI
Typical periods offered: Spring

CHEM 5580 Special Topics in Organic Chemistry
This course focuses on an important current topic in organic chemistry. Open to undergraduates with the permission of the instructor.
Credit 3 units.
Typical periods offered: Fall

CHEM 5590 Organic Chemistry Seminar
The organic chemistry graduate students enrolled will each present one seminar on a topic of current interest in the literature.
Credit 1 unit.
Typical periods offered: Fall, Spring

CHEM 5610 Inorganic Chemistry
Inorganic chemistry encompasses the structure, properties, and reactivity of inorganic molecules and solids. This course will focus on the symmetry, bonding, electronic structure, spectroscopy, and reactivity of inorganic coordination complexes in which ligands are bound to one or more metal centers. The course will start with using group theory to classify molecules based on the symmetry elements they possess. A series of different bonding models including VSEPR, valence bond theory, molecular orbital theory, crystal field theory, and ligand field theory will be used to describe the structure and bonding of inorganic molecules, coordination complexes, and organometallic compounds. These models will serve as a basis for interpreting and predicting the electronic and vibrational spectra of inorganic compounds.
Credit 3 units. A&S IQ: NSM Art: NSM
Typical periods offered: Fall

CHEM 5612 Advanced Inorganic Chemistry
Study of physical inorganic concepts with an emphasis on modern experimental methods applied to inorganic and bioinorganic systems. The spectral and magnetic properties of inorganic and bioinorganic compounds will be discussed. Topics in group theory will be covered, including symmetry of molecules and ions, the application of group theory in molecular structure determination, chemical bond theory and spectroscopy for inorganic materials as molecular species and in crystal lattices. Prerequisite: Chem 461, or consent of instructor.
Credit 3 units.

CHEM 5613 Group Theory
The course will develop applications of group theory to MO theory for inorganic compounds, ligand-field theory, spectral transition probabilities, molecular vibrations, and vibronic coupling.
Credit 3 units.

CHEM 5620 Solid-State and Materials Chemistry
A description of how the structures of crystalline solids at different length scales control their chemical and physical properties is critical for understanding how these materials are applied in a variety of technologies ranging from solar cells to lithium batteries. This course begins with basic crystallography and introduces common inorganic structure types as well as common defects in crystalline solids. With the aid of computer models, students will learn to analyze and index x-ray powder-diffraction patterns that provide a fingerprint to identify a crystal. The relation between the crystal structure of a solid and its resulting electronic structure, chemical reactivity, and physical properties (e.g., optical, electrical, and mechanical) will be discussed throughout the semester with an emphasis on how crystal defects alter these properties. The course will conclude with the use of phase diagrams to assess the composition and microstructure of metals and ceramics. Prerequisite: Chem 105/111A or permission of instructor
Credit 3 units. A&S IQ: NSM Art: NSM

CHEM 5630 Inorganic Electrochemistry and Photochemistry
An understanding of electrochemical processes is critical in describing the behavior of batteries, fuel cells, and other important devices used in energy conversion and environmental remediation. This course will cover modern inorganic electrochemistry, photochemistry, and photoelectrochemistry from a microscopic perspective of solid-electrolyte interfaces. The course material will start with the thermodynamics of solid-electrolyte interfaces and the kinetics of electron transfer across these interfaces. Electroanalytical techniques, including cyclic voltammetry and potential-step experiments, will be described to understand the mechanism of electrochemical and photochemical reactions. Lectures will include applications of electrochemical cells in catalysis, materials synthesis, and solar-fuel generation. Prerequisites: Chem 461, or Chem 465, or consent of instructor.
Credit 3 units. A&S IQ: NSM Art: NSM

CHEM 5670 Inorganic Chemistry Laboratory
A laboratory course emphasizing both the synthesis of inorganic compounds and the study of their physical properties. Laboratory exercises will introduce novel synthetic techniques including high-temperature synthesis and vacuum-line manipulations. Compounds will be spectroscopically characterized by UV-visible absorption, gas-phase infrared, and multinuclear and dynamic NMR spectroscopies. Measurements of electrochemical behavior, magnetic susceptibility, and electrical conductivity will be performed. Prereq: Chem 461 or consent of the instructor. A Writing Intensive option is available with the permission of the instructor.
Credit 3 units. A&S IQ: NSM Art: NSM
Typical periods offered: Spring

CHEM 5680 Special Topics in Inorganic Chemistry
This course focuses on an important current topic in inorganic chemistry. Prior completion of Inorganic Chemistry is recommended.
Credit 3 units.

Typical periods offered: Fall, Spring

CHEM 5690 Inorganic/Organometallic Chemistry Seminar
Students present informal seminars on topics of current interest from the chemical literature or from their own dissertation research.
Credit 1 unit.
Typical periods offered: Fall, Spring

CHEM 5810 General Biochemistry I
Topics include the properties and structures of biomolecules, including amino acids, nucleotides, lipids, carbohydrates, proteins and nucleic acids. Additional topics include enzyme kinetics and mechanisms, membrane structure and properties, protein folding, an introduction to metabolism, oxidative phosphorylation and photosynthesis. This course is the first semester of an integrated two-semester sequence.
Credit 3 units. A&S IQ: NSM Art: NSM
Typical periods offered: Fall

CHEM 5811 Introduction to Biomolecules
The goal of this course is to introduce students to the preparation, characterization, structure-function relationship, and chemistry of proteins, polysaccharides, and nucleic acids. The course emphasizes understanding the chemical and physical properties of the respective building blocks and their noncovalent interactions as the foundation for macromolecular properties and function. Students will apply fundamental energetic and mechanistic principles (from general and organic chemistry) and develop chemical reasoning skills that enable scientific problem-solving towards the understanding of chemical phenomena in biological systems.
Credit 3 units.
Typical periods offered: Fall

CHEM 5820 General Biochemistry II
Biochemistry explores the chemistry of life processes at the molecular level. This course is the second semester of a two-semester General Biochemistry sequence. The first semester of the Biochemistry sequence covered the basics of the topic with an emphasis on the structures, functions, and interactions of biomolecules including proteins, nucleic acids, carbohydrates, and lipids. This second semester course will emphasize metabolism, the biosynthetic (anabolism) and degradation (catabolism) pathways that provide the energy of life and define the molecules associated with healthy and disease states.
Credit 3 units. A&S IQ: NSM Art: NSM
Typical periods offered: Spring

CHEM 5821 Chemical Biology
This course is a survey of modern chemical biology focusing on the application of a broad array of chemical tools to biological problems. The course is roughly divided into four sections; biopolymers, computational methods and bioinformatics, tools for chemical biology, and applications of chemical biology. A mandatory discussion section accompanies the course and is used to review current and classical literature in the field. Prereqs: Chem 262 and Biol 2970, or permission of the instructor.
Credit 3 units. A&S IQ: NSM Art: NSM

CHEM 5830 Bioorganic Chemistry
This course presents a molecule-centered perspective on the current state of the art in antibiotic drug discovery and natural products chemistry. The molecular mechanisms of antibiotic drug action and pathogen resistance will be covered along with the biosynthetic origins of antibiotics from plants and microbes. The course is taught from the perspective of understanding how organic chemistry plays out in biological systems, with an emphasis on small organic molecules and enzymes. Curved arrow mechanisms will be used frequently in learning activities and assignments. A working knowledge of protein structure and function is helpful. Students are encouraged (but not required) to take General Biochemistry I and/or General Biochemistry II in preparation for this course. Students will be responsible for writing a review article on an assigned antibiotic molecule and presenting their paper to the class.
Credit 3 units. A&S IQ: NSM Art: NSM
Typical periods offered: Fall

CHEM 5831 Nucleic Acids
Credit 3 units. A&S IQ: NSM Art: NSM

CHEM 5833 Protein Biochemistry
The focus of this course is protein biochemistry, and is intended to build upon General Biochemistry. In this course we will focus on protein structure, folding, and techniques to purify and characterize protein activity. We will progress from initial studies to first understand protein fold and function to current efforts to better characterize protein structure-function relationships. We will also highlight human diseases that are underpinned by protein misfolding. This course will focus on reading and understanding primary literature, including landmark papers along with more recent work. During the second half of the semester, each student will select a paper and prepare a written analysis of that paper. The student will then present the paper and lead a journal club style discussion of the paper.
Credit 3 units. A&S IQ: NSM Art: NSM BU: SCI
Typical periods offered: Spring

CHEM 5840 Simulation in Chemistry and Biochemistry
This course explores a wide range molecular modeling techniques and applications of computational chemistry to problems in chemistry and biochemistry. Topics include ab initio quantum mechanics, semi-empirical MO theory, molecular mechanics, molecular dynamics simulation, coarse-grained models, electrostatic methods and biomolecular structure prediction. A major component of the course is weekly laboratory sessions using common software programs in the field, including Spartan, Q-Chem, Gaussian, VMD, TINKER, APBS, AutoDock, SDA7 and others. Many of the lab exercises target proteins, nucleic acids and other biological structures. As a final lab experience, students will complete an independent project using tools covered in the course.
Credit 3 units. A&S IQ: NSM Art: NSM

CHEM 5841 Chemical Dynamics of Biological Pathways
This course will provide a highly advanced evaluation of cellular metabolism. The course will interrogate metabolic pathways and associated enzymatic mechanisms by tracking stable isotope labeling patterns as measured by liquid chromatography/mass spectrometry. The course will not contain any background treatment of mass spectrometry or basic metabolism. To be enrolled, students must already have an in-depth understanding of these topics. Major objectives of the course are: (1) to learn how to use labeling patterns qualitatively to understand chemical mechanisms at the arrow-pushing level as well as metabolic regulation, (2) to learn metabolic flux analysis, (3) to understand the complex metabolic interactions between cells and organs, and (4) to understand how metabolic reprogramming of specific cell types supports physiologic coordination at the organismal level. Pre-reqs: Chem 482/Chem 5820/Biol 4820 AND permission of instructor.
Credit 3 units.
Typical periods offered: Spring

CHEM 5843 Mass Spectrometry
The first focus of the course is an overview of the subject and its history. The second covers the fundamentals of ionization to produce molecular ions. Ionization methods include electron ionization, chemical ionization, electrospray, and matrix-assisted laser desorption. Thermodynamic principles of ionization including ionization energies, proton affinities, and gas-phase acidities provide a fundamental basis for ionization. The third major focus is interpretation of EI and product-ion spectra from MS/MS. Mechanisms of gas-phase ion decomposition reactions, rates and thermodynamics of gas-phase ion processes, and ion-molecule reactions are discussed in terms of interpreting spectra. A major emphasis is the spectra of peptides and proteins, providing a basis for the field of proteomics and related omics areas. The fourth focus is the fundamentals of instrumentation design and implementation: quadrupole, time-of-flight, ion trap, orbitraps, and Fourier transform instruments. Combined or hyphenated GC/MS, LC/MS, and tandem mass spectrometry are also discussed. Applications in a variety of areas are worked in as the course progresses: structure determination of synthetic, natural products, metabolites, and biomolecules, exact mass measurements (high resolution MS), peptide and protein and other biomolecule sequencing, sensitive detection, trace analysis, and mixture analysis. Prerequisite: Chem 262 or permission of instructor.
Credit 3 units.
Typical periods offered: Spring

CHEM 5890 Biological Chemistry Seminar
This course is required for all graduate students following the biological chemistry track. The course will consist of tutorials for first year graduate students and research presentations by second year students. Prerequisites: enrollment in the biological chemistry track or permission of the instructor.
Credit 1 unit.
Typical periods offered: Fall, Spring

CHEM 5900 Research
Hours to be arranged.
Credit 0.5-9 units.
Typical periods offered: Fall, Spring

CHEM 595 Drug Delivery Systems: Principles and Applications
Credit 3 units.

CHEM 7000 Master's Continuing Student Status
Credit 0 units.

CHEM 7010 Master's Nonresident
Credit 0 units.

CHEM 7020 Master's Resident
Credit 0 units.

CHEM 8000 Doctoral Continuing Student Status
Credit 0 units.

CHEM 8010 Doctoral Nonresident
Credit 0 units.

CHEM 8020 Doctoral Resident
Credit 0 units.