CHE

Chemistry

CHE 501: Instrumental Methods in Chemistry
Practical and theoretical aspects of instrumentation in chemistry. The primary emphasis is on contemporary methods of molecular structure determination such as X-ray crystallography, NMR, IR, and MS. Other topics may also be presented.
Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 502: Mechanisms and Strategies in Organic Synthesis
This course will focus on (1) the meaning and practice of writing organic reaction mechanisms and (2) standard synthetic reactions, their mechanisms, and modern refinements. Examples and applications will be presented. The course will also discuss biomimetic syntheses and the use of mechanism in designing total syntheses.
Fall, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 503: Synthetic Organic Chemistry
A survey of the most important organic reactions from the viewpoint of synthetic utility, including many recent innovations in this field. Throughout the discussion of these methods, emphasis is placed upon their use in the synthesis of complex organic structures.
Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 504: Structure and Reactivity in Organic Chemistry
Electronic and stereochemical theories relating to organic structure and reactions. Topics such as bonding, strain, aromaticity, MO theory, molecular rearrangements, pericyclic reactions, and photochemistry are covered. This course is intended to provide a foundation of knowledge at the beginning graduate level as preparation for advanced subjects in CHE 502 and CHE 503, and is complementary to CHE 501.
Fall, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 505: Structural Inorganic Chemistry
Properties and reactions of inorganic compounds are considered from the viewpoint of molecular and electronic structure. The modern bonding theories used in inorganic chemistry including molecular orbital, valence bond, and ligand field theories are developed using symmetry and group theory. Selected main group, transition metal, and organometallic compounds are discussed. An introduction to crystallography and solid-state structure is included.
Fall, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 514: Transition Metal Chemistry
A survey course with an emphasis on the transition metals. Reaction mechanisms, synthesis, and structure are covered. Specific areas of concern include coordination chemistry, organometallic chemistry, bioinorganic chemistry, and selected topics from solid-state and non-transition metal chemistry.
Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 515: Advanced Inorganic Chemistry
A topical course with an emphasis on the current literature. Subject matter varies and is announced in advance. Possible subjects include reaction mechanisms, organometallic chemistry, bioinorganic chemistry, and physical inorganic chemistry. May be repeated as the subject matter varies.
Spring, 3 credits, Letter graded (A, A-, B+, etc.)
May be repeated for credit.

CHE 516: Solid-State Chemistry
This course will provide an introduction to structure and bonding in solid materials. This class will survey the important structural classes of periodic solids and will discuss space groups and the crystallographic symmetry elements important to these materials. Topics that will be covered may include, but are not limited to: (i) The mechanisms by which crystals grow and common types of defects. (ii) An introduction to the basics of band theory. (iii) An overview of the important synthetic methods for preparing solid state materials in nanocrystalline, powder, thin film, and single crystal form. (iv) A survey of the important techniques for assessing the composition, homogeneity, and crystallinity of materials (such as SEM, TEM, AFM, STM), with an emphasis on powder x-ray diffraction.
Fall, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 517: Structural Chemistry
Much of chemistry is concerned with the properties of atoms and molecules that are too small to see directly. This course will cover a variety of advanced techniques for elucidating the atomic-scale structure of molecules and periodic solids. A central technique is diffraction, which probes periodic arrays. The mathematical basis for diffraction will be presented, followed by practical examples of obtaining atomic coordinates from diffraction data (powder and/or single crystal). Other techniques that may be covered include the analysis of local structure in partially ordered or disordered solids (via techniques such as PDF, EXAFS, small angle scattering, or solid state NMR), and the basis of more complex diffraction experiments (neutron/ electron diffraction, energy-dispersive/Laue diffraction, and diffraction under extreme pressure/temperature conditions).
Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 518: Materials Chemistry
Our high technology world is driven forward by advances in materials chemistry. This class will discuss the origin of this technology, covering the synthesis, structures, and properties of advanced materials. These materials will be studied from a multidisciplinary perspective, since the knowledge required for their development spans more than one traditional academic discipline. This class will focus on broad topics with great current societal importance (energy, computing, nanoscience, etc.), and will discuss the materials at the heart of our present technology as well as novel classes of materials being developed for future technology applications. Specific topics may include batteries, fuel cells, catalysts, metallic conductors, semiconductors, superconductors, permanent magnets, magnetic films.
Co-listed with CHE 378
Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 521: Quantum Chemistry I
Quantum theoretical concepts are discussed. Schrodinger wave mechanics and related mathematical techniques are illustrated by treatment of systems of chemical interest. Designed to form the theoretical basis for the study of chemical bonding, molecular structure, spectroscopy, and molecular collision phenomena.
Fall, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 522: Molecular Spectroscopy
A detailed description of the theory and practice of molecular spectroscopy. Topics include the interaction of molecules with electromagnetic radiation and the time evolution of molecular energy states.
Prerequisite: CHE 521
Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 523: Chemical Thermodynamics
A rigorous development of the fundamentals of thermodynamics and its application to a number of systems of interest to chemists, such as electrochemical cells, gases, and homogeneous and heterogeneous equilibrium. An introduction to statistical mechanics will also be included.

Fall, 1-3 credits, Letter graded (A, A-, B+, etc.)

CHE 524: Magnetic Resonance
This course provides an introduction to the fundamental quantum mechanics of the magnetism of spin-1/2 (and higher) particles. It includes a study of the Bloch equations (the responses of the magnetism to continuous-wave and pulsed irradiation) and a discussion of the experimental hardware and techniques commonly employed. Topics covered include the basics of the spin Hamiltonian (chemical shifts, J, dipolar, and quadrupolar couplings), dynamics and relaxation 1-D spectroscopy (spin and chemical exchange, lineshapes, spin echoes, etc.), 2-D spectroscopy (homonuclear and heteronuclear correlation), techniques for studies of solids and liquid crystals (magic angle spinning, cross polarization, quadrupolar echo), and the principles of magnetic resonance imaging. Applications to the biological and material sciences, as well as chemical problems, will be discussed.

Spring, alternate years, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 525: Theoretical Chemistry
This course stresses the physical theory underlying chemical phenomena. Special emphasis is given to advanced topics in electronic structure theory, molecular dynamics, condensed matter and surfaces, many-body and quantum ensemble theory, and the interaction of light and molecules.

3 credits, Letter graded (A, A-, B+, etc.)

CHE 528: Statistical Mechanics
Statistical theory of equilibrium systems and rate processes. Ensemble theory, spatial and time correlation functions. Model systems and methods of estimating their properties. Designed to enable the student to use the current literature dealing with application of statistical mechanics to problems in chemistry.

Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 530: Physical Chemistry of Macromolecules
An investigation of the gross and fine structures of macromolecules and molecular aggregates in solution as revealed by hydrodynamic behavior (e.g., ultracentrifugation, viscosity), light scattering, spectroscopic properties (e.g., ultraviolet hypochromism, circular dichromism, Raman, fluorescence, magnetic resonance spectra), and the thermodynamics and kinetics of interaction with small molecules and ions. Theory of conformation changes and phase transitions.

3 credits, Letter graded (A, A-, B+, etc.)

CHE 535: Introduction to Computational Structural Biology and Drug Design
This course will provide an introduction to Computational Structural Biology with application to Drug Design. Methods and applications that use computation to model biological systems involved in human disease will be emphasized. The course aims to foster collaborative learning and will consist of presentations by the instructor, guest lecturers, and by course participants with the goal of summarizing key methods, topics, and papers relevant to Computational Structural Biology.

Fall, 0-3 credits, Letter graded (A, A-, B+, etc.)

CHE 536: Molecular Modeling of Biological Molecules
This course is designed for students who wish to gain hands-on experience modeling biological molecules at the atomic level. In conjunction with the individual interests, Molecular Mechanics, Molecular Dynamics, Monte Carlo, Docking (virtual screening), or Quantum Mechanics software packages can be used to study relevant biological system(s). Projects will include setup, execution, and analysis. Course participants will give literature presentations relevant to the simulations being performed and a final project report will be required. Familiarity with UNIX (Linux) is desirable.

Prerequisite: CHE 535 or permission of instructor

Spring, 0-3 credits, Letter graded (A, A-, B+, etc.)

CHE 541: Biomolecular Structure and Analysis
The structures of biological macromolecules and the relationship of their structure to biological function are described. Methodology employed to study macromolecules is also discussed. Topics include chemical and physical properties of cell and tissue constituents, including carbohydrates, lipids, nucleic acids, proteins and peptides. Prerequisite: Strong foundation in physical and organic chemistry.

Fall, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 542: Chemical Biology
The reactivity and physiological function of biological macromolecules and their cofactors are described at the chemical biochemical level. The emphasis of this course reflects recent advances in chemical biology. Possible topics include catalysts, reaction mechanisms, correlation between three-dimensional structure and reactivity, receptor-ligand interactions in extracellular and intracellular signaling, protein folding in vitro and in vivo.

Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 543: Chemical Approaches to Biology
The use of molecular concepts and methodology to solve problems in biology and medicine. The course covers methods to elucidate and control biological systems. Possible topics include chemical genomics, metabolomics, and chemotherapeutics.

Prerequisite: CHE 542

Fall, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 558: Physical Biology
This is a course on the principles of physical chemistry. We describe the nature of the forces and energies and entropies that drive molecular systems toward their states of equilibrium.

We consider a broad range of applications throughout chemistry, biology, materials engineering and nanoscience. This course aims to give students an understanding of how the actions and behaviors of materials arise from their atomic and molecular structures.

Co-listed with PHY 558

Spring, 3 credits, Letter graded (A, A-, B+, etc.)

CHE 559: Biological Dynamics and Networks
This course will provide a solid foundation in key theoretical concepts for the study of dynamics in biological systems and networks at different scales ranging from the molecular level to metabolic and gene regulatory networks. Topics of this course include but are not limited to: Physical kinetics; Diffusion/Smoluchowski; Random flights; Waiting times; Poisson; Brownian ratchets; Chemical kinetics; Transition states; Stability, bifurcations, pattern development; Noise in cells: intrinsic and Extrinsic; Feedback; Biological Oscillators; Recurrence, period doubling, chaos; Networks; Topologies; Degree distribution, betweenness; Models of nets: Erdos-Renyi, scale-free, social, Watts-Strogatz, agents; Robustness, highly-optimized tolerance, bowties, epidemics; Biological networks: Protein-protein nets, regulatory and metabolic nets; Known biological circuits and their behaviors; How networks evolve:
Includes current trends in chemical research and the influence of chemistry in areas such as the environment and technology. Topics of local interest and the conflicting demands placed on technology will be integrated into the course. Offered in Fall.
3 credits, Letter graded (A, A-, B+, etc.)

CHE 593: Chemical Demonstrations
The design and implementation of demonstrations to illustrate modern concepts of chemistry.
3 credits, Letter graded (A, A-, B+, etc.)

CHE 595: Scientific Computing
The basic methods of numerical analysis as well as the design of computer programs that use them are discussed within the framework of solving a variety of exciting problems chosen from all areas of science. The presentation makes extensive use of powerful scientific computational environments, such as Mathematica and Matlab, but guidance to other scientific high-level computer languages is also provided. No previous knowledge of computer programming is assumed.
2 credits, Letter graded (A, A-, B+, etc.)

CHE 598: Professional Masters Internship
Participation in private corporations, public agencies, or non-profit institutions for research and other experiential training activities related to the completion of a Master term paper. Students will be required to have a faculty coordinator as well as a contact in the outside organization, to participate with them in regular consultations on the project, and to successfully complete CHE 590. Prerequisites: Permission of Master's Program Director. 0-12 credits, S/U grading May be repeated for credit
Offered
Fall, Spring, and Summer, 0-12 credits, S/U grading May be repeated for credit.

CHE 599: Research
Fall, Spring, 1-12 credits, S/U grading May be repeated for credit.

CHE 602: Special Topics in Physical Organic Chemistry
The subject matter varies depending on interests of students and staff. It may cover such areas as photochemistry, theoretical organic chemistry, and the chemistry of unstable intermediates; the emphasis is on fundamental considerations and recent developments.
1-12 credits, Letter graded (A, A-, B+, etc.) May be repeated for credit.

CHE 603: Special Topics in Bioorganic Chemistry
The subject matter varies depending on interests of students and faculty. Possible topics include asymmetric synthesis and natural product synthesis.
Fall, 1-3 credits, Letter graded (A, A-, B+, etc.) May be repeated for credit.

CHE 605: Advanced Organic Chemistry
The subject matter varies depending on interests of students and staff. Possible topics include organic synthesis and natural product synthesis.
Fall, 1-3 credits, Letter graded (A, A-, B+, etc.) May be repeated for credit.
Experimental methods in the determination of molecular structure. The emphasis is on the determination of structure in the solid state, particularly by X-ray crystallography. Students complete a single-crystal molecular structure determination using modern diffractometer techniques.

3 credits, Letter graded (A, A-, B+, etc.)

**CHE 641: Organometallic Chemistry**
A systematic presentation of the chemistry of organometallic compounds, particularly those of the transition metals. Topics include structure, bonding, reaction mechanisms, synthesis, and applications in catalysis and organic synthesis.

3 credits, Letter graded (A, A-, B+, etc.)

**CHE 682: Special Topics in Inorganic Chemistry**
Subject matter varies, depending on interests of students and staff, but covers recent developments in inorganic chemistry.

0-3 credits, Letter graded (A, A-, B+, etc.)
May be repeated for credit.

**CHE 683: Special Topics in Physical Chemistry**
Subject matter varies, depending on interests of students and staff, but covers recent developments and advanced topics in physical chemistry.

3 credits, Letter graded (A, A-, B+, etc.)
May be repeated for credit.

**CHE 690: Internship in Dissertation-Related Research**
Supervised curricular training in dissertation-related research. Prerequisite: For full-time: Summer session or advancement to candidacy; Permission of Graduate Program Director.

Fall and Spring, 1-3 credits, S/U grading
May be repeated for credit.

**CHE 693: Physical Chemistry Seminar**
Fall and Spring, 0-12 credits, S/U grading
May be repeated for credit.

**CHE 694: Biological Chemistry Seminar**
Fall and Spring, 0-12 credits, S/U grading
May be repeated for credit.

**CHE 695: Inorganic Chemistry Seminar**
Fall and Spring, 0-12 credits, S/U grading
May be repeated for credit.

**CHE 696: Organic Chemistry Seminar**
Fall and Spring, 0-12 credits, S/U grading
May be repeated for credit.

**CHE 697: Seminar in Physical and Quantitative Biology**
Fall and spring, 0-1 credits, S/U grading.
0-1 credits, S/U grading
May be repeated 1 times FOR credit.

**CHE 698: Colloquium**
Fall and Spring, 0-12 credits, S/U grading
May be repeated for credit.

**CHE 699: Dissertation Research on Campus**
Prerequisite: Must be advanced to candidacy (G5). Major portion of research must take place on SBU campus, at Cold Spring Harbor, or at the Brookhaven National Lab.
Fall, Spring, and Summer, 1-9 credits, S/U grading
May be repeated for credit.

**CHE 700: Dissertation Research off Campus - Domestic**
Prerequisite: Must be advanced to candidacy (G5). Major portion of research will take place off-campus, but in the United States and/or U.S. provinces. Please note, Brookhaven National Labs and the Cold Spring Harbor Lab are considered on-campus. All international students must enroll in one of the graduate student insurance plans and should be advised by an International Advisor.
Fall, Spring, 1-9 credits, S/U grading
May be repeated for credit.

**CHE 701: Dissertation Research off Campus - International**
Prerequisite: Must be advanced to candidacy (G5). Major portion of research will take place outside of the United States and/or U.S. provinces. Domestic students have the option of the health plan and may also enroll in MEDEX. International students who are in their home country are not covered by mandatory health plan and must contact the Insurance Office for the insurance charge to be removed. International students who are not in their home country are charged for the mandatory health insurance. If they are to be covered by another insurance plan they must file a waiver by second week of classes. The charge will only be removed if other plan is deemed comparable.
All international students must received clearance from an International Advisor.
Fall, Spring, 1-9 credits, S/U grading
May be repeated for credit.

**CHE 800: SUMMER RESEARCH**
May be repeated for credit.