Chemistry (CHE)

Chair: Benjamin S. Hsiao, Chemistry Building Room 104, (631) 632-7885
Graduate Program Director: Nancy S. Goroff, Chemistry Building Room 741, (631) 632-8356
Student Affairs Coordinator: Katherine M. Hughes, Chemistry Building Room 104, (631) 632-7886

Degrees awarded: M.S. in Chemistry; Ph.D. in Chemistry

The Department of Chemistry, within the College of Arts and Sciences, offers courses of study leading to the degrees of Master of Arts in Teaching Chemistry, Master of Science, and Doctor of Philosophy. Students in the M.A.T. program must register through the School of Professional Development. A student in the Ph.D. program may choose dissertation research in any one of the diverse areas of chemistry represented by the interests of the program faculty, or may choose an interdisciplinary topic under the guidance of a faculty member in another program. Coordinated activities exist with several programs, and include optional concentrations in chemical physics and chemical biology.

Facilities

The Chemistry Building is a modern, seven-story (170,000-sq.-ft.) structure designed for research and upper-division instructional activities. The equipment available to faculty, postdoctorals, and students is outstanding. While much of it has been commercially obtained, a substantial portion of the instrumentation of the Department has been designed and constructed at Stony Brook and represents the state of the art in various fields. Strong ties exist to programs at Brookhaven National Laboratory, with unique facilities in PET and magnetic resonance imaging, the Relativistic Heavy Ion Collider, the National Synchrotron Light Source, the Center for Functional Nanomaterials, and world-class programs in dynamics, materials science, and spectroscopy.

The construction and maintenance of this instrumentation is effected by the faculty in conjunction with a staff of nonteaching professionals in the electronic, glass, and machine shops. Our nuclear magnetic resonance (NMR) and computer facilities are staffed by an NMR coordinator and a computer coordinator, respectively.

Areas of Current Research

Synthetic Chemistry

The synthesis of new molecular compounds distinguishes chemistry from other scientific disciplines. Although many disciplines study the properties of materials and natural phenomena, only chemistry concerns itself with the preparation of new molecular arrangements. The success of past synthetic efforts can readily be appreciated by observing the vast array of new materials that have improved the quality of our lives.

The Department of Chemistry at Stony Brook is very fortunate to have many strong synthetic programs in both organic and inorganic chemistry. Among the studies underway are the search for inventive synthetic reactions to produce new molecules, the synthesis of new molecular structures to evaluate our theories of chemical bonding, and the synthesis of new compounds with unusual physical properties (molecular engineering). However, most of the synthetic interest in the program lies in the areas of bio-organic and bio-inorganic chemistry. Synthetic chemistry is being applied to the understanding of receptor-substrate interactions as well as of enzyme function, the preparation of artificial enzymes, the mechanism of mutagenesis and carcinogenesis, and the preparation of new compounds for the treatment of patients.

Organometallic Chemistry

Organometallic chemistry is an interdisciplinary field bringing together many aspects of inorganic and organic chemistry. A wide range of organometallic systems are under study using a variety of synthetic, structural, mechanistic, and theoretical techniques. Synthetic and structural research is focused on such problems as the chemistry of unsaturated metal-carbon bonds in metal carbene and carbyne complexes, the stabilization of highly reactive organic moieties through metal complexation, the chemistry of transition metal carbonyl cluster compounds, and the development of useful synthetic reagents. Homogeneous catalysis studies include investigations of the carbonylations of fluoroolefins, small-ring heterocycles, alkenylamides, and similar molecules, and catalytic applications of compounds with unsaturated metal-carbon bonds. Theoretical work includes ab initio and qualitative molecular orbital studies of organometallic compounds and of the chemisorption of organic molecules onto metal surfaces and molecular mechanics minimizations of ligand geometries.

Structural and Mechanistic Organic Chemistry

The structures of a wide range of organic molecules are examined at Stony Brook using many techniques, including automated high-field FT-NMR spectroscopy (1H, 13C, 19F, etc.) and X-ray crystallography. Molecular modeling programs, such as Macromodel, are operated on color graphics workstations in order to rationalize and predict the conformations and reactivities of molecules under study. Variable-temperature 1H and 13C NMR spectroscopy is used to investigate conformational changes in macrocycles and other synthetic hosts for guest metal ions and organic molecules. VT-NMR is also used to investigate proton transfer in polyamines and intermolecular exchange of guest ions between polydentate ligands. Stereochemical probes are used to examine mechanisms of organic reactions such as pericyclic and biomimetic processes, and have provided proof of the existence of sigma-participation in reactions of unstrained ketones and carbonium ions. Reaction mechanisms are also studied by determining activation volumes using reactors in the high-pressure laboratory that can attain pressures higher than 200,000 psi.

Institute of Chemical Biology and Drug Discovery (ICB&DD)

The primary objective of ICB&DD, directed by Distinguished Professor Iwao Ojima, is to establish a world-class "Center of Excellence" in chemical biology and drug discovery at Stony Brook. The rapid and impressive advancement of chemical biology in the last decade clearly demonstrated that solutions for a vast majority of medical problems rely on the understanding of the molecular basis of diseases, therapeutic targets, drug actions, and drug resistance. ICB&DD promotes highly productive interdisciplinary and collaborative research among chemists, biologists, medicinal chemists, pharmacologists, and physicians to attack major and significant biomedical problems to find solutions including the discovery of novel therapeutic drugs.

Biological Chemistry

A significant number of the faculty are using their chemical expertise to explore the chemical and physical details of biological phenomena. Research programs span biological chemistry, biophysics, enzyme mechanisms, membrane structure and function, protein folding, and structural biology. Techniques such as high-resolution NMR, stop-flow kinetics, fluorescence and Raman spectroscopy are used to probe protein structure, function, and folding. Novel biosynthetic and chemical strategies are being used to generate small molecules for use in probing enzyme mechanisms and exploring ligand-receptor interactions.

Inorganic Chemistry

Inorganic chemistry, being concerned with the synthesis, structure, and dynamics of the compounds formed by the more than 100 natural and synthetic elements, covers an extremely vast area of chemistry. New compounds and new synthetic methods are among the goals of inorganic chemistry. Such compounds range from materials important in technology to catalysts for industrial chemical processes, small molecules present in outer space, and metal complexes that serve as models for biological materials. The methodologies utilized in inorganic chemistry include a wide variety of spectroscopic techniques, kinetic methods, procedures for the elucidation of geometric and electronic structures, and theory. The breadth and depth of inorganic chemistry are well represented at Stony Brook, as seen by the following examples of current research: thermally and photochemically activated dynamic processes, in particular, electron transfer reactions; synthetic and structural studies of active site analogs of metalloenzymes such as the zinc proteins that regulate gene transcription and the high-potential iron-sulfur proteins; activation of small molecules by transition metal complexes and homogeneous catalysis; chemistry of unsaturated carbon-metal bonds in mononuclear compounds and in extended molecular assemblies; molecular orbital calculations and molecular mechanics methods applied to transition metal cluster compounds and related organometallic substances; NMR studies of zeolites and supported catalysts.

Magnetic Resonance

Magnetic resonance in the Department of Chemistry ranges from studies in physiology to studies in chemical physics. Topics under investigation include the use of liquid and solid state NMR spectroscopy and micro-imaging techniques with stable spin 1/2 and quadrupolar nuclides to study inorganic, organic, biological, and living systems. Projects in progress employ a range of single and N-dimensional NMR spectroscopic techniques and novel imaging techniques to elucidate chemical processes and determine the structures of biological and organic molecules in solution.

Novel NMR methods are being developed for the determination of the structures of micro- and macromolecules as they exist in disordered solids and to study the structure and dynamics of molecules in the liquid crystalline state and those absorbed on solid surfaces. Pulsed electron paramagnetic resonance (EPR) techniques are being developed to study metalloenzymes, organic conductors, and other molecules.

The NMR facility in the Department of Chemistry includes seven NMR spectrometers, a multinuclear, research grade, 600 MHz (14.1 T) spectrometer with 3-axis field gradient capability and a standard 51 mm bore magnet for liquids and solids CP/MAS spectroscopy, a multinuclear, research grade, 500 MHz (11.75 T) spectrometer with z-axis field gradient capability and a standard 51 mm bore magnet for liquids spectroscopy, a multinuclear research grade spectrometer at 400 MHz (9.4 T) with an 89 mm wide bore magnet that is available for imaging and solids spectroscopy, a 300 MHz (7.0 T) spectrometer with a z-axis gradient for routine liquid NMR spectroscopy, a multinuclear 250 MHz (5.88 T) standard bore magnet spectrometer that is also available for routine NMR spectroscopy, and two wide bore spectrometers dedicated to solids.

Macromolecules

With development of state-of-the-art X-ray diffraction and small-angle X-ray scattering (SAXS) at the State University of New York's X3 Beamline at the National Synchrotron Light Source at Brookhaven National Laboratory, the polymer and biomacromolecular physics group, being members of the participating research team (PRT), possesses one of the most powerful X-ray scattering facilities in the country. The experiments at Stony Brook make use of a wide variety of complementary techniques such as SAXS, laser light scattering, photon correlation spectroscopy, fluorescence photobleaching recovery, holographic relaxation spectroscopy, transient electric birefringence, and various forms of NMR spectroscopy. Stony Brook scientists can perform measurements to determine the structure and dynamical behavior of advanced polymeric materials, supramolecular systems, and biomacromolecules. Time-dependent processes can be studied using stop-flow, steady-flow, pressure-jump, and temperature-jump experiments together with time-resolved capabilities using intense radiation sources such as pulsed lasers and the synchrotron radiation. Unparalleled opportunities exist for interdisciplinary research using unique and novel instrumentation in polymer materials, polymer physics, colloid science, and biophysical chemistry.

Photon-Molecule Interactions

Recent developments in the use of lasers for the investigation of molecular structure and dynamics have led to a revolution in the fields of molecular spectroscopy and dynamics. Intimate details about the structure and interactions of atoms and molecules can now be studied to an extent never before possible. In this program the systems being studied by laser spectroscopy range from atoms and diatomic molecules to molecular crystals and polymers. In these systems various properties are being investigated, including nonlinear interactions with the radiation field, excited state electronic structure, radiationless transitions, ionization mechanisms, crystal field interactions, and photochemical reactions, as well as electron and energy transfer processes. Luminescence spectroscopy, luminescence excitation, multiphoton ionization, multiphoton photoelectron spectroscopy, Raman spectroscopy, and vacuum ultraviolet spectroscopy are among the techniques being used and developed for the ever greater understanding of atomic and molecular systems.

Soft X-Ray Spectroscopy

The National Synchrotron Light Source at Brookhaven National Laboratory, located only 15 miles from Stony Brook, provides unique opportunities for frontier research in chemistry. The synchrotron and associated devices are unequaled sources of high-intensity X-ray and vacuum ultraviolet radiation. One area of current research uses soft X-rays, photons with energies of 100 to 1000 eV, to investigate the excitation and relaxation of core electrons in molecules. Because core electrons, e.g., the 1s electrons of carbon, are tightly bound to individual atoms, the excitation energy is essentially localized on a particular atom in the molecule. This localization has the potential for producing photochemistry with far greater atomic site specificity than can be achieved by excitation of valence electronics with visible and ultraviolet light.

Surface Chemistry

Catalysis, corrosion, and friction are a few examples of familiar processes that occur on solid surfaces. The field of surface chemistry tries to unravel and understand the basic chemical principles that underlie such phenomena. At Stony Brook we are actively researching how the electronic and geometric structure of a surface affects its chemical selectivity and reactivity during surface-mediated processes such as catalysis and the chemical vapor deposition of metals from organometallic precursors. In addition, we are interested in understanding the interactions between energetic ions and surfaces in both atmospheric and metal-etching reactions. An arsenal of sophisticated techniques is available to prove both the geometric and electronic structures of a reacting surface on an atomic level. Techniques such as Auger electron spectroscopy (AES) and high-resolution, electron energy loss spectroscopy (HREELS) are used to determine the composition of a surface, while ultraviolet and X-ray photons are commonly used to eject photoelectrons from a surface (that are energy analyzed) yielding electronic structure information. Another technique, low-energy electron diffraction (LEED), exploits the wave nature of electrons and is used to help determine the geometric structure of a surface. These techniques, routinely used at Stony Brook, are complemented by the powerful extended- and near-edge X-ray absorption fine-structure techniques (EXAFS and NEXAFS), available at the National Synchrotron Light Source at nearby Brookhaven National Laboratory.

Theoretical Chemistry

Theoretical investigations of a wide variety of chemical phenomena are underway at Stony Brook. Research programs in electronic structure theory are concerned with the development of formalism and computational techniques. Applications include determination of the geometry, spectral shifts, and reaction pathways of molecules chemisorbed onto metal surfaces; calculation of the structure of molecules in highly excited Rydberg states; and evaluation of probability amplitudes for multiphoton excitation and calculation of Born corrections, Born couplings, and orbital stresses in small molecules. In the field of statistical mechanics, analysis and numerical simulation are combined to obtain properties of liquids and ionic solutions from the properties of their constituent molecules and their interactions. Much of this work is focused on the calculation of pair correlation functions, transport properties and dielectric phase diagrams, solvent effects, and rates of electron transfer reactions. Other current work includes theory of photon-molecule interactions, quantum ensembles, Jahn-Teller dynamics, and lifetimes of quasistationary molecular states. In addition, students often do theoretical work closely related to active experimental programs under the joint guidance of a theorist and an experimentalist.

Nuclear and Isotope Chemistry

Nuclear chemistry research at Stony Brook has focused on reactions induced by heavy ion beams. Beams are obtained from accelerators located at Stony Brook, Berkeley, Chicago, Michigan, and France. The reactions produce very hot and rapidly rotating atomic nuclei that are studied by observation of particles and fragments that are emitted. Their energies and angles of emission allow for a reconstruction of the properties of the hot emitting nuclei and the mechanism of their production.

Isotope chemistry deals with the small differences in physical and chemical properties of matter that have their origin in the mass difference of isotopes of an element. Although the effects are small, they can be measured with high precision. In general, the effects are quantum effects, and measurement of isotope effects has proven to be a unique method for the study of molecular and intermolecular forces. Isotope effect studies have found application in chemical physics, organic chemistry and biochemistry, geochemistry, and anthropology. Practical applications are found in isotope separation processes. Our present efforts are concentrated on the systematization of isotope chemistry.

Admission

The following, in addition to the minimum Graduate School requirements, are required for admission to graduate study in chemistry:

A. A bachelor's degree in chemistry earned in a curriculum approved by the American Chemical Society, or an equivalent course of study;

B. A minimum grade point average of 3.00 (B) in all undergraduate work and 3.00 (B) in all courses in the sciences and mathematics;

C. Results of the Graduate Record Examination (GRE) General Test;

D. Acceptance by the Department of Chemistry and by the Graduate School.

In exceptional cases, a student not meeting requirements A and B may be admitted on a provisional basis.

Faculty

Distinguished Professors

Bigeleisen, Jacob, *Distinguished Professor Emeritus*, Ph.D., 1943, University of California at Berkeley: Statistical mechanical theory of isotope chemistry.

Chu, Benjamin, Ph.D., 1959, Cornell University: Laser light scattering; synchrotron X-rays; rheometry; laser induced fluorescence; nano-microstructures and supramolecular formation in polymer colloids; complexation in photoelectrolytes and surfactants; capillary electrophoresis; supercritical fluids; molecular composites; blends and fibers.

Ojima, Iwao, Ph.D., 1973, University of Tokyo, Japan: Development of new and effective methodologies for the syntheses of bioactive compounds of medicinal interest based on organic and organometallic chemistry; medicinal chemistry and chemical biology of anticancer agents, MDR reversal agents, and enzyme inhibitors.

Stell, George R., *Distinguished Research Professor*, Ph.D., 1961, New York University: Statistical thermodynamics; molecular theory of fluids; theories of gelation and polymerization.

Professors

Alexander, John M., Ph.D., 1956, *Emeritus*, Massachusetts Institute of Technology: Reactions between complex nuclei; use of detected ejectiles to characterize super-heated emission sources.

Drueckhammer, Dale G., Ph.D., 1987, Texas A&M University: Bioorganic chemistry; computer-guided design in molecular recognition, design and synthesis of receptors and sensors for biological molecules; chemistry and enzymology of coenzyme A.

Fowler, Frank W.,[1] Ph.D., 1967, University of Colorado: The development of methods for the preparation of supramolecular assemblies and their application to problems in material science.

Grey, Clare P., D.Phil., 1991, Oxford University, England: Materials chemistry; solid-state NMR spectroscopy; characterizing and studies of anionic conduction in fuel cell membranes and structure of battery materials; environmental chemistry; modifying reactive sites in catalysts.

Haim, Albert,[2] *Emeritus*, Ph.D., 1960, University of Southern California: Kinetics and mechanisms of inorganic reactions.

Hanson, David M., Ph.D., 1968, California Institute of Technology: Design and development of classroom learning structures; text-based and Web-based learning systems; and course assessment systems.

Hsiao, Benjamin S., Ph.D., 1987, University of Connecticut: Polymer physics; polymer crystallization; structure and property relationships in nanostructured polymers; nanocomposites and biodegradable polymer; polymers for biomedical applications; synchrotron X-ray scattering and diffraction.

Ishida, Takanobu, *Emeritus*, Ph.D., 1964, Massachusetts Institute of Technology: Isotope effects, stable isotope separation, electrochemistry of nitrogen oxides and carbon oxides in biological fluids.

Johnson, Francis,[3] Ph.D., 1954, Glasgow University, Scotland: Structure and total synthesis of naturally occurring biologically active molecules; DNA damage and enzymatic repair mechanisms; new synthetic methods in organic synthesis; heterocyclic chemistry.

Johnson, Philip M., Ph.D., 1967, Cornell University: Optical molecular spectroscopy and the electronic structure of molecules; development of spectroscopic techniques using high powered lasers.

Kerber, Robert C.,[4] *Distinguished Teaching Professor*, Ph.D., 1965, Purdue University: Chemical education; esp. effects of terminology on learning; history of chemistry.

Koch, Stephen, Ph.D., 1975, Massachusetts Institute of Technology: Synthesis and structure in transition metal coordination chemistry; metal ions in biological systems; early transition metal catalysts.

Lacey, Roy A.,[5] Ph.D., 1987, University at Stony Brook: Nuclear chemistry; intermediate and relativistic energy heavy ion reaction studies.

Lauher, Joseph W.,[6] Ph.D., 1974, Northwestern University: Structural chemistry; design and synthesis of new inorganic and organic materials; hydrogen bonding; molecular graphics; X-ray crystallography.

le Noble, William J., *Emeritus*, Ph.D., 1957, University of Chicago: Stereoelectronics with applications such as nucleophilic and electrophilic addition, oxidation and reduction, metal complexation, pericyclic reactions and the reverse processes; reactions in compressed solutions.

London, Erwin,[7] Ph.D., 1979, Cornell University: Lipid-protein and protein-protein interactions in membranes; membrane protein folding and translocation by membrane penetrating toxins; cholesterol and lipid domain formation.

Mayr, Andreas, Ph.D., 1978, University of Munich, Federal Republic of Germany: Reactivity of metal-carbon multiple bonds; synthesis of molecular components for nanocomputing.

Parise, John B.,[8] Ph.D., 1981, University of North Queensland, Australia: Synthetic solid-state chemistry; structural chemistry; crystallography; materials research.

Parker, Kathlyn A., Ph.D., 1971, Stanford University: Organic synthesis; synthetic methods; natural products, non-natural nucleosides; designed enzyme inhibitors; molecular tools for biochemistry.

Raleigh, Daniel P., Ph.D., 1988, Massachusetts Institute of Technology: Biological chemistry; experimental studies of protein folding and protein stability; studies of amyloid formation; NMR studies of protein dynamics.

Sampson, Nicole S., Ph.D., 1990, University of California, Berkeley: Enzyme mechanisms and protein-protein interactions; the use of organic synthesis, kinetics and mutagenesis to probe the structure and function of enzymes and cell-surface recognition proteins.

Tonge, Peter J., Ph.D., 1986, University of Birmingham, England: Biological chemistry and enzyme mechanisms; quantitating substrate strain in enzyme-substrate complexes using vibrational spectroscopy; rational drug design.

White, Michael, Ph.D., 1979, University of California, Berkeley: Surface chemical dynamics; catalysis; photo-induced reactions; molecular spectroscopy; molecular beam scattering.

Associate Professors

Goroff, Nancy, Ph.D., 1994, University of California, Los Angeles: Design and synthesis of carbon-rich organic molecules and materials; halocumulenes and alkynes; three-dimensional chromophores for biological fluorescence studies; cyclophenacenes ("buckybelts") and other unusual conjugated systems.

Millar, Michelle M., Ph.D., 1975, Massachusetts Institute of Technology: Reactivity, electronic, and structural properties of transition metal complexes; organometallic chemistry; bio-inorganic chemistry.

Schärer, Orlando D.,[3] Ph.D., 1996, Harvard University: Chemical biology of mammalian DNA repair.

Schneider, Robert F.,[11] Ph.D., 1959, Columbia University: Chemical education; Web-based instruction; laboratory instruction.

Simmerling, Carlos, Ph.D., 1994, University of Illinois, Chicago: Computational chemistry and structural biology; molecular dynamics of biological macromolecules.

Wong, Stanislaus, Ph.D., 1999, Harvard University: Nanoscience; physical chemistry; biophysical chemistry; materials science; scanning probe microscopy imaging of nanomaterials; synthesis and characterization of nanostructures such as nanocrystals and nanotubes; physical, chemical, and biological applications of nanotechnology.

Wishnia, Arnold, Ph.D., 1957, New York University: Physical chemistry of biological macromolecules; structure and function of ribosomes; membrane model systems; applications of nuclear magnetic resonance.

Assistant Professors

Boon, Elizabeth, Ph.D., 2002, California Institute of Technology: Biochemistry; prokaryotic nitric oxide biology and the role of the H-NOX family; peptide and protein engineering for novel sensing applications.

Carrico, Isaac, Ph.D., 2003, California Institute of Technology: Chemical biology and bio-organic chemistry; introduction of unnatural amino acids and sugars into cell and virus systems for diagnostic and therapeutic purposes; development of new reactions designed to take place inside living systems.

Jia, Jiangyong, Ph.D., 2003, Stony Brook University: Ultra-relativistic heavy ion reaction studies.

Khalifah, Peter, Ph.D., 2001, Princeton University: Solid state chemistry; electronic and magnetic materials; renewable energy; X-ray diffraction; crystal growth.

Wang, Jin, Ph.D., 1991, University of Illinois: Physics and chemistry of biomolecules; single molecule reaction dynamics.

Adjunct Professors

Fowler, Joanna, Ph.D. 1968, University of Colorado: Organic synthesis with short-lived positron-emitting isotopes; neuroscience; drug mechanisms; brain imaging.

Marecek, James F., Ph.D., 1971, Case Western Reserve University: Chemical synthesis.

Rodriguez, Jose A., Ph.D., 1988, Indiana University: Surface chemistry and catalysis.

Sears, Trevor John, Ph.D., 1979, Southampton University, England: Gas phase laser spectroscopy; frequency modulation; free radical spectroscopy; molecular structure and dynamics; small metallic clusters.

Adjunct Assistant Professors

Green, David, Ph.D., 2002, Massachusetts Institute of Technology: Computational biology of protein interactions.

Raineri, Fernando O., Ph.D., 1987, University of Buenos Aires: Theoretical chemistry; solvent effects on electron transfer reactions; equilibrium and nonequilibrium solvation; thermodynamics, structure and dynamics of liquids and solutions.

Rizzo, Robert C., Ph.D., 2001, Yale University: Quantifying molecular recognition with quantitative structural biology.

Number of teaching, graduate, and research assistants, Fall 2007: 165

1) Recipient of the State University Chancellor's Award for Excellence in Teaching, 1995

2) Recipient of the State University Chancellor's Award for Excellence in Teaching, 1981

3) Joint appointment, Department of Pharmacology

4) Recipient of the State University Chancellor's Award for Excellence in Teaching, 1986; Recipient of the President's Award for Excellence in Teaching, 1986

5) Recipient of the State University Chancellor's Award for Excellence in Teaching, 1998; Recipient of the President's Award for Excellence in Teaching, 1998

6) Recipient of the State University Chancellor's Award for Excellence in Teaching, 1990; Recipient of the President's Award for Excellence in Teaching, 1990

7) Joint appointment, Department of Biochemistry

8) Joint appointment, Department of Geosciences

9) Recipient of the State University Chancellor's Award for Excellence in Teaching, 2001; Recipient of the President's Award for Excellence in Teaching, 2001

Degree Requirements

Requirements for the M.S. Degree in Chemistry

A. Successful completion of an approved course of study comprising at least 30 credits of graduate coursework. A student must achieve a 3.0 overall grade point average in all courses taken at Stony Brook to receive a degree.

B. Successful completion of the CHE 532 seminar and six courses made up from any of the following groups: CHE 501 through 530, 541, 542, 557 through 589, 601 through 604, 623 through 683, and approved courses offered through other programs or through the School of Professional Development (SPD).

C. Successful completion of the CHE 590 term paper or research, thesis, and thesis defense.

Requirements for the M.A. Degree in Teaching Chemistry

The curriculum for a Master of Arts in Teaching Chemistry consists of 36 credits distributed among graduate-level course offerings in chemistry, other sciences and mathematics, teaching methods in both science and general education, and practice teaching in secondary schools. Individual programs are tailored to the background and interests of the student in consultation with an advisor.

Requirements for the Ph.D. Degree in Chemistry

A. Courses

Successful completion of an approved course of study comprising at least six formal graduate courses of which four are selected from CHE 501 through 550, in addition to CHE 531, 532, and two semesters of Teaching Practicum (CHE 610, 611) or the equivalent is required. The following courses are recommended for inclusion among the six formal courses, distributed from among at least two of the following four groups: Group I–one of CHE 521, 522, 523, 528; Group II–one of CHE 511, 514, 515; Group III–one of CHE 501, 502, 503, 504; Group IV–one of CHE 530, 541, 542. Continuation in the Ph.D. program is based, in part, on achievement in four 500-level Chemistry courses to be taken during the student's first year. In consultation with faculty advisors each student selects a course of study to acquire a good background for research in the area of Chemistry chosen.

B. Advancement-to-Candidacy (Preliminary) Examination

A student is advanced to candidacy for the Ph.D. degree when all degree requirements except the dissertation have been completed. A special committee is designated for each student to aid in progressing toward this step. The committee is charged with advising the student and administering the advancement-to-candidacy (preliminary) examination. This examination, normally completed within two years following qualification to the Ph.D. degree, consists of a written proposition and oral defense, a discussion of the student's research, and discussion or evaluation of the recent literature.

C. Presentation of a Departmental Seminar

D. Research, Dissertation, Dissertation Defense, and Departmental Colloquium

Each student selects a faculty research advisor at some time after the middle of the first semester and usually before the middle of the second semester. The research advisor also serves on the advancement-to-candidacy committee.

Specific inquiries from prospective graduate students regarding research opportunities are welcomed and should be addressed to the chair. The *Graduate Programs in Chemistry* brochure states in some detail the varied research interests of the Chemistry faculty and is available from the Department.

E. Residence

A one-year residence is required.

F. Teaching

Three semesters of teaching experience are required. In some cases, research activity may be substituted in lieu of one semester of teaching.

Requirements for the Ph.D. Degree, Concentration in Chemical Physics

A field of concentration in Chemical Physics is provided for students whose interests lie in both chemistry and physics. A graduate student who is admitted to either the Department of Chemistry or the Department of Physics may elect this course of study with the consent of the Department chair. A Chemistry student elects this course of study to obtain more extensive training in physics than is normally required by chemistry programs. A Physics student elects this concentration to obtain more extensive exposure to chemical systems than is normally obtained in physics programs. A student in the Chemical Physics concentration may select a research advisor from either program subject to the approval of the chairs.

For a Chemistry student the requirements are the same as for the Ph.D., with the following exceptions.

A. Courses

CHE 531, 532, two semesters of CHE 610 or 611, and six graduate courses are required, including the following:

1. CHE 523 Chemical Thermodynamics
2. Either CHE 521 Quantum Chemistry I or PHY 511 Quantum Mechanics I
3. One course from among CHE 501, 502, 504, 511, 514, 515, 541, 542 (Organic/Inorganic/Biological Chemistry)
4. Three courses from among CHE 522, 524, 525, 526, 527, 528, 529, and 530 and PHY 501, 503, 505, 540, 551, 555, and 565. Other graduate courses can be substituted only with prior permission of the graduate advisement committee. A prerequisite for the Chemical Physics program is undergraduate training in classical mechanics and electromagnetic theory at or above the level of PHY 301 Electromagnetic Theory and PHY 303 Mechanics. Students in Chemical Physics must take these courses unless they receive waivers from the graduate advisement committee.

B. Advancement-to-Candidacy (Preliminary) Examination

In some cases a hybrid of the Chemistry and Physics requirements may be used.

Requirements for the Ph.D. Degree, Concentration in Biological Chemistry

The field of concentration in biological chemistry is a course option for students whose interests lie in both chemistry and biology. A graduate student who is admitted to the Department of Chemistry or another appropriate program may elect this field of concentration with the consent of the graduate coordinator. The course of study can provide more extensive training in biology than is normally required for a Chemistry graduate degree and more extensive exposure to fundamental chemical studies for students in other programs. In addition, a student may select a research advisor in any appropriate program, subject to the approval of the Chairs involved.

A. Courses

CHE 531, two semesters of CHE 610 or 611, and six graduate courses are required, including the following:

1. Two courses from among CHE 501-530.
2. A minimum of two graduate biology/biochemistry-oriented courses (for example, BMO 520, BMO 512, CHE 541, CHE 542) as approved by the graduate advisement committee. Students will normally take CHE 541 and 542. A prerequisite for the Biological Chemistry Program is undergraduate training in biology or biochemistry at or above the level of BIO 361 Biochemistry I. Students in the Biological Chemistry program must take this course unless they receive a waiver from the graduate advisement committee.

B. Advancement-to-Candidacy (Preliminary) Examination

Must complete two semesters each of CHE 619 and 694. These courses replace CHE 532 and other literature presentation requirements for advancement to candidacy.

Courses

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, ABCF grading

CHE 502 Mechanistic Organic Chemistry

Important reaction mechanisms and the methods by which they are studied. Substituent and medium effects on reactions proceeding through concerted mechanisms and unstable intermediates are discussed.
Spring, 3 credits, ABCF grading

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, ABCF grading

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, ABCF grading

CHE 511 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, ABCF grading

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, ABCF grading

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.
Spring, 3 credits, ABCF grading
May be repeated for credit

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, ABCF grading

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, ABCF grading

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, 3 credits, ABCF grading

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 echos, 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, ABCF grading

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.
Prerequisite: CHE 521
3 credits, ABCF grading

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, ABCF grading

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, ABCF grading

CHE 531 Departmental Research Seminar
Meetings in which first-year graduate students learn about the research activities of the Departmental faculty.
Fall, 0 credit, S/U grading

CHE 532 Literature Seminar
Students select and discuss topics from the current literature.
Spring, 0 credit, ABCF grading

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. Crosslisted with AMS 535.
Fall, 0-3 credits, ABCF grading

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. Crosslisted with AMS 536.
Prerequisite: CHE 535 or permission of instructor
Spring, 0-3 credits, ABCF grading

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, ABCF grading

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, ABCF grading

CHE 589 Directed Study
Subject matter varies according to needs of student.
Fall and spring, 0-12 credits, ABCF grading
May be repeated for credit

CHE 590 M.S. Term Paper
Independent study leading to a term paper on a selected topic in chemistry, chemical applications, or chemical pedagogy.
Fall and spring, 3 credits, ABCF grading

CHE 591 Chemistry in Society
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.
Fall, 3 credits, ABCF grading

CHE 593 Chemical Demonstrations
The design and implementation of demonstrations to illustrate modern concepts of chemistry.
3 credits, ABCF grading

CHE 599 Research
Fall and spring, 1-12 credits, S/U grading

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, ABCF grading
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, ABCF grading
May be repeated for credit

CHE 606 Special Topics in Synthetic Chemistry
1-3 credits, ABCF grading
May be repeated for credit

CHE 610 Practicum in Teaching
Practice instruction in chemistry at the undergraduate level, carried out under faculty orientation and supervision. A minimum of two semesters of CHE 610 or 611 is required of all candidates for graduate research degrees in chemistry, unless explicitly waived by the Chair.
Fall and spring, 1-3 credits, ABCF grading
May be repeated for credit

CHE 611 Practicum in Teaching
Practice instruction in chemistry at the undergraduate level, carried out under faculty orientation and supervision. A minimum of two semesters of CHE 610 or 611 is required of all candidates for graduate research degrees in chemistry, unless explicitly waived by the Chair.
Fall and spring, 0 credit, ABCF grading
May be repeated

CHE 619 Critical Readings of Current Topics in Chemistry
Recent research papers from the literature will be analyzed in depth. These papers may originate from the inorganic, organic, physical, and/or biochemical literature. The exact topic of the course is announced in advance.
Fall and spring, 0-3 credits, ABCF grading
May be repeated for credit

CHE 625 Molecular Structure and Crystallography
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, ABCF grading

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, ABCF grading

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, ABCF grading
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, ABCF grading
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

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

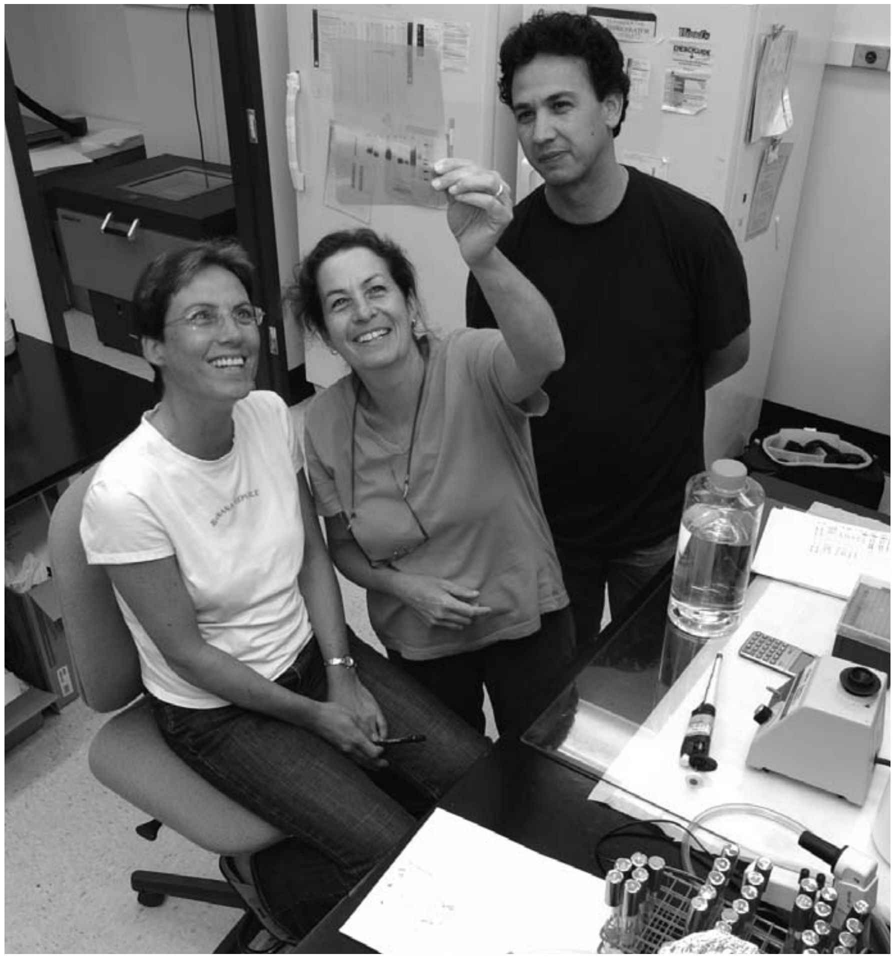
CHE 695 Inorganic Chemistry Seminar
Fall and spring, 0-12 credits, S/U grading
May be repeated for credit

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

CHE 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 SB campus, at Cold Spring Harbor, or at 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 U.S. and/or U.S. provinces (Brookhaven National Lab and 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, and summer, 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 the U.S. 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 the second week of classes; the charge will be removed only if the other plan is deemed comparable); all international students must receive clearance from an International Advisor
Fall, spring, and summer, 1-9 credits, S/U grading
May be repeated for credit

CHE 800 Summer Research
0 credit, S/U grading
May be repeated for credit