### Chemistry Department

### Chairperson

Peter J. Tonge, Chemistry Building 779 (631) 632-5797

## **Graduate Program Director**

Isaac Carrico, Chemistry Building 533 (631) 632-7935

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### **Degrees Awarded**

M.S. in Chemistry; Ph.D. in Chemistry

#### Web Site

http://www.stonybrook.edu/commcms/chemistry/

#### **Application**

https://graduateadmissions.stonybrook.edu/apply/

#### Chemistry Department

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.

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 Chemistry Department 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). A major focus 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 diseases.

#### **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 Gaussian and 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. 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 & Drug Discovery at Stony Brook (ICB&DD)

The primary objective of the ICB&DD, directed by Distinguished Professor Iwao Ojima, is to serves as 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 demonstrates that solutions for the vast majority of medical problems rely on the understanding of the molecular basis of diseases, therapeutic targets, drug actions, and drug resistance. The 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, enzyme mechanisms, protein folding, membrane structure and function, biophysics 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 research area. New compounds and new synthetic methods are among the goals of inorganic chemistry research. 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 used 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 Chemistry Department ranges from studies in physiology to studies in chemical physics. Topics under investigation include the use of liquid and solid state nuclear magnetic resonance (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 Stony Brook NMR Facility http://www.stonybrook.edu/commcms/nmr/ is a campus-wide facility that serves the educational and research needs of the University community. With spectrometers located at two different sites, the Chemistry Department and the Center for Molecular Medicine (CMM), the NMR facility offers instrument access to students, post-docs and investigators on diverse research fields including structural biology, chemistry, biophysics, and material sciences. The facility has been updated recently with new Bruker spectrometers, and has a total of nine instruments operating from 300 to 850 MHz proton frequencies.

#### 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 nuclear magnetic resonance 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 underly 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 (which 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 requirements of Chemistry Department

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.

Facilities of Chemistry Department

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 spectroscopy, dynamics and materials science.

The construction and maintenance of this instrumentation is effected by the faculty in conjunction with a staff of non-teaching professionals in the electronic, glass, and machine shops. Our nuclear magnetic resonance (NMR) facility is staffed by two NMR coordinators.

# Requirements for the M.S. Degree in Chemistry

There are three different options for completing the M.S. degree in Chemistry at Stony Brook. The standard M.S. degree is based on coursework and the writing of a term paper that presents a critical review of a current topic in chemistry. We also offer an M.S. degree with a concentration in Chemical Research. For this option, students need to complete less coursework, but must also carry out a minimum of 18 credits of research, and must write and defend an original research thesis. The third option, the M.S. in Chemistry with concentration in Professional Science, offers students the opportunity to combine chemistry training, including a full-year internship, with additional professional courses in business, management, and/or communication.

### Requirements for the Standard 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 GRD 500, the CHE 582 seminar (B-), and 18 credits of formal scientific courses (B- = 2.67 average) selected from among chemistry graduate courses, and approved courses from other departments. The student must complete a minimum of 3 core 500-level chemistry courses, from among those numbered CHE 501 through 559. All course selections must be approved by the Master's Advising Committee.

C. Successful completion of the CHE 590 term paper.

# Requirements for the M.S. Degree with Concentration in Chemical Research

- 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 CHE 581, GRD 500, the CHE 582 seminar (B-), and at least 12 credits of formal scientific courses (B- = 2.67 average) selected from among chemistry graduate courses, and approved courses from other departments. The student must complete a minimum of 3 core 500-level chemistry courses, from among those numbered CHE 501 through 559. All course selections must be approved by the Master's Advising Committee.
- C. Chemistry research, including a minimum of 18 research credits (18 credits of CHE 599 or 15 credits of CHE 599 plus 3 credits of the summer research course CHE 597), culminating in successful completion of a research thesis with public defense, describing a body of original research results. The thesis defense committee, assigned by the Graduate Program Director, will include the research advisor and two other Chemistry program faculty, one of whom will serve as committee Chair.

### Requirements for the M.S. Degree with Concentration in Professional Science

- 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 GRD 500 and at least 12 credits of formal scientific courses (B— = 2.67 average) selected from among chemistry graduate courses, and approved courses from other departments. The student must complete a minimum of 3 core 500-level chemistry courses, from among those numbered CHE 501 through 559. All course selections must be approved by the Master's Advising Committee.
- C. Successful completion of 9 credits of additional professional coursework ("plus" courses) in areas such as business, management, writing, or journalism.
- D. Successful completion of at least 18 credits of laboratory internship (CHE 598). Internship placements will be determined by the Master's Advising Committee, in consultation with the student, typically at the end of the first academic year. The Professional Science concentration offers internships in a variety of laboratory settings, including government labs (BNL), industrial labs, and regional research consortiums.
- E. Successful completion of the CHE 590 term paper.

## 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 Bachelor of Science Degree/Master of Science Degree Program

A student interested in this research-intensive graduate program, intended to prepare students for professional employment in the chemical or pharmaceutical industries, may apply for admission at the end of the junior year. The program leads to a Bachelor of Science degree in Chemistry at the end of the fourth year and a Master of Science in Chemistry at the end of the fifth year. During the senior year, the student is expected to take two 500-level CHE courses and begin research in the senior research sequence. In the fifth year, the student works full-time on research, earning 24 credits in CHE 599.Current Stony Brook undergraduate students majoring in chemistry, biochemistry, or engineering chemistry are eligible to apply for admission to the Bachelor of Science Degree/Master of Science Degree Program.

## Requirements for the Ph.D. Degree in Chemistry

## A. Courses

Successful completion (3.0 GPA) of eighteen credits in formal graduate courses (including CHE 599 rotation research, but excluding seminars, teaching, directed study, etc.). At least nine of these credits must be from courses numbered CHE 501 through 559, and at least twelve credits must be from courses in Chemistry. Courses are designated among the following four subdisciplinary groups: Group I – Physical Chemistry: CHE 521, CHE 522, CHE 523, CHE 524, CHE 528, CHE 530; Group II – Inorganic Chemistry: CHE 511, CHE 514, CHE 515, CHE 516, CHE 517, CHE 518; Group III – Organic Chemistry: CHE 501, CHE 502, CHE 503, CHE 504, CHE 607; Group IV – Biological Chemistry: CHE 535, CHE 536, CHE 541, CHE 542, CHE 543. Students are required to take at least one course outside their major subdiscipline. Continuation in the Ph.D. program is based, in part, on achievement in at least four chemistry courses to be taken during the student's first year. In addition, students are required to complete CHE 581; CHE 582; CHE 619 (unless the student elects to complete Option 1 for the Second Meeting requirement);

GRD 500; CHE 693, 694, or 696; and two semesters of Teaching Practicum (CHE 610, CHE 611). Initially, each student will be assigned an academic advisor to help the student select an appropriate course of study to prepare for research in the student's chosen area of chemistry. Once a student has joined a research group, the research advisor acts as academic advisor.

Students who have taken equivalent courses previously may be excused from individual course requirements with permission of the Graduate Program Director, in consultation with the Graduate Advising Committee.

## **B.** Advancement to Candidacy Committee

Each student selects a faculty research advisor during the first year. Students begin research during the first year or in the summer directly following. At the start of the second year, the Graduate Program Director will assign the student's Advancement to Candidacy Committee (ACC). In addition to the research advisor, the ACC will also include at least two additional Chemistry program faculty, one of whom will serve as Chair of the committee.

### C. Qualification to Degree

In the third semester, each student holds the first formal meeting with his or her ACC. At the end of this First Meeting, the ACC makes a recommendation to the faculty of whether the student should be qualified to the Direct Ph.D. track or the MS Thesis track, or needs to leave the program. This recommendation will be based on the student's research performance, knowledge and understanding as demonstrated during the First Meeting, and course grades. Qualification is determined by the faculty as a whole. Students must have satisfactory performance in research and coursework in order to qualify to either track and remain in the Ph.D. program.

The ACC will also consider whether the student has gaps in knowledge or understanding that should be addressed by further coursework. The student may be directed to take additional courses, beyond the minimum requirement.

#### Direct Ph.D. Track

Students with satisfactory research performance and science course GPA above 3.0 will generally be qualified to the Ph.D. Direct Track. These students can continue with research and complete the other requirements for the Ph.D., without needing to complete a MS thesis first.

## M.S. Thesis Track

Students with science course GPA below 3.0 or deficiencies in understanding or research progress, as determined during the ACC First Meeting, may be qualified to the MS Thesis Track. A student in the MS Thesis track must complete a master's thesis as a first step in the Ph.D. program. Upon completion and defense of the MS thesis, such a student must petition the faculty to continue in the Ph.D. program. If the petition is approved, the student will then join the Direct Ph.D. track and will need to fulfill all requirements of that track in order to earn the Ph.D.

# D. Second ACC Meeting

During the fourth semester, students will complete the requirement for a Second Meeting with the ACC. This requirement can be met in several ways. Students in physical, inorganic, or materials chemistry or in chemical physics will generally follow Option 1 or Option 2. Students carrying out research in organic chemistry and in biological chemistry will generally follow Option 2.

# Option 1

The second meeting shall consist of an oral report on one or two papers from the recent literature. This report should demonstrate a mastery of the problems and methodology covered in the material. The role of the Advancement to Candidacy Committee is to assess the quality of the report and also to assess the student's intellectual growth. Further study may be recommended at this time.

# Option 2

The student will enroll in the appropriate section of CHE 619 *Critical Readings of Current Topics in Chemistry* (organic chemistry; biological chemistry; physical/inorganic/materials chemistry), and will make a presentation in the class during the second year. This presentation will be in addition to any presentation the student makes in CHE 582 during the first year.

# E. Advancement to Candidacy

Once a student in the Direct Track has successfully completed his or her coursework and First and Second Meetings with the ACC, the student will be advanced to candidacy. From that point forward, the student will focus on research.

# F. Department Seminar

Every Ph.D. student in the Direct Track will present a departmental seminar in the third year, describing his or her research. Starting in the third year, students in organic chemistry will be expected to present their research annually in CHE 696, while biological chemistry students will present their research annually in CHE 694 through their fifth year in the program. All other students will present a single research seminar in the fall of the third year, in CHE 693.

### G. Research Proposition and Third ACC Meeting

At least one year before the anticipated thesis defense, the student will prepare an original research proposition and defend the proposition in a closed meeting with the ACC. The proposition is a research proposal based on the literature rather than on the student's own research. At the Third Meeting, the student and committee will also discuss the student's research progress and exit plan for completing the dissertation. A target

date for the defense will be set at the conclusion of the Third Meeting. The Third Meeting report may also be used in place of a CHE 590 term paper for any student who wishes to obtain a Master's degree.

#### H. Dissertation Defense

The ACC serves as the basis for the dissertation defense committee, with the addition of one new member from outside the department. The dissertation and defense must adhere to all policies of the Graduate School. The defense will be a public lecture, followed by private examination by the defense committee.

## Requirements for the Ph.D. Degree with Concentration in Chemical Physics

#### A. Courses

CHE 581, 582, GRD 500, and two semesters of CHE 610/611 plus six formal graduate courses (including CHE 599 rotation research, but excluding seminars, teaching, directed study, etc.) are required including the following:

- 1. CHE 523, Chemical Thermodynamics
- 2. Either CHE 521 (Quantum Chemistry I) or PHY 511 (Quantum Mechanics I)
- 3. Three courses from a set approved by the Graduate Advisement Committee. This set consists of CHE 522, 524, 525, 528, 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 Program Director.
- 4. One additional course from outside of Group I.

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 the Chemical Physics program must take these courses unless they receive waivers from the Graduate Program Director.

### **B.** Additional Requirements

Other than coursework, the requirements for the Ph.D. in Chemical Physics are the same as those for the Ph.D. in Chemistry.

## Requirements for the Ph.D. Degree with Concentration in Biological Chemistry

#### A. Courses

CHE 581, GRD 500, and two semesters of CHE 610/611 plus 18 credits of formal graduate courses (including CHE 599 rotation research, but excluding seminars, teaching, directed study, etc.), including

- 1. A minimum of two graduate biology/biochemistry oriented courses (e.g., BMO 520, CHE 541, CHE 542, etc.) as approved by the student's Academic Advisor or ACC. Students will normally take CHE 541, CHE 542, and CHE 543.
- 2. At least one course from outside of Group IV.
- 3. Registration for CHE 582 (year one, zero units), CHE 619 (year two, maximum two units) and CHE 694 (years three through five, one unit) in the Spring semesters of the first five years of the program (while still in residence). Students in their first and second year will present a research paper from the literature. Students in their third and fourth years (and fifth year if still in residence) will present a seminar on their thesis research.

# **B.** Additional Requirements

Other than coursework, the requirements for the Ph.D. in Biological Chemistry are the same as those for the Ph.D. in Chemistry,

Faculty of Chemistry Department

### **Distinguished Professors**

Dill, Kenneth, Distinguished Professor, Ph.D., 1978, University of California: Statistical mechanics and dynamics of biological systems.

Hsiao, Benjamin S., Distinguished Professor, 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.

Lauher, Joseph W.<sup>1</sup>, Distinguished Teaching Professor, Ph.D., 1974, Northwestern University: Structural chemistry; design and synthesis of new inorganic and organic materials; hydrogen bonding; molecular graphics, x-ray crystallography.

London, Erwin<sup>2</sup>, Distinguished Professor, 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.

Ojima, Iwao, Distinguished Professor, 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.

Parise, John B.<sup>3</sup>, Distinguished Professor, Ph.D., 1981, University of North Queensland, Australia: Synthetic solid-state chemistry; structural chemistry; crystallography; materials research.

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

Sampson, Nicole S., Distinguished Professor, 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.

Takeuchi, Esther, <sup>4</sup> Distinguished Professor and William and Jane Knapp Endowed Chair in Energy and the Environment, Ph.D., 1981, The Ohio State University: Fundamental chemistry and electrochemistry of energy storage, synthesis and characterization of electrochemically active materials; nanomaterials and nanostructured materials related to energy storage.

Takeuchi, Kenneth<sup>5</sup>, Distinguished Teaching Professor, Ph.D., The Ohio State University: Energy storage; fundamental chemistry and electrochemistry of energy storage, synthesis and characterization of electrochemically active materials; nanomaterials and nanostructured materials related to energy storage.

Tonge, Peter J., Distinguished Professor, 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.

Wong, Stanislaus S., <sup>6</sup> Distinguished Professor, Ph.D., 1999, Harvard University: Nanoscience; physical chemistry; inorganic 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.

#### **Professors**

Bhatia, Surita, Ph.D., 2000, Princeton University: Rheology and phase behavior of associative polymer gels; small-angle scattering; structure and rheology of colloidal dispersions and complex fluids; polymeric materials for cell encapsulation, delivery, and wound healing.

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.

Chapman, Karena. Professor of Chemistry and Joseph W. Lauher and Frank W. Fowler Endowed Chair in Materials Chemistry, Ph.D., 2005, University of Sydney: Solid state materials, energy storage and conversion, structure-property relationships, crystallography, catalysis, metalorganic frameworks, synchrotron-based characterization, functional materials, X-ray scattering.

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.

Goroff, Nancy, Ph.D., 1994, University of California, Los Angeles: Design and synthesis of carbon-rich organic molecules and materials; halocumulenes and alkynes; 3-dimensional chromophores for biological fluorescence studies; cyclophenacenes ("buckybelts") and other unusual conjugated systems.

Grubbs, Robert B., Ph.D., 1998, Cornell University: Polymer chemistry; block copolymer materials; polymer assemblies; controlled radical polymerization.

Jia, Jiangyong, Ph.D., 2003, State University of New York at Stony Brook: Ultra-relativistic heavy ion reaction studies.

Johnson, Francis, 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.

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

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., 8 Ph.D., 1987, University at Stony Brook: Nuclear chemistry; intermediate and relativistic energy heavy ion reaction studies.

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

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.

Sears, Trevor John, Ph.D., 1979, Southampton University, England: High resolution spectroscopy of transient species; molecular structure; development of new instrumental techniques; gas phase free radical dynamics and kinetics.

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

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

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

#### **Associate Professors**

Aubrecht, Katherine, Ph.D., 1999, Cornell University: Chemical education, education for sustainability, context-based chemistry education, sustainable polymeric materials.

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.

Laughlin, Scott, Ph.D., 2008, University of California, Berkeley: chemical biology, neuroscience, organic chemistry.

Ngai, Ming-Yu, Ph.D., 2008, University of Texas at Austin: Organic and organometallic chemistry, photochemistry, radiochemistry, and biomedical imaging.

Rudick, Jonathan G., Ph.D., 2005, University of Pennsylvania: Organic, supramolecular, and polymer chemistry.

### **Assistant Professors**

Allison, Thomas, <sup>9</sup> Ph.D., 2010, University of California, Berkeley: Chemical Physics. Frequency combs. Ultrasensitive femtosecond spectroscopy, and high-order harmonic generation.

Boros, Eszter, Ph.D. 2011, University of British Columbia: Radiochemistry, inorganic chemistry and chemical biology; development of metalbased diagnostics and therapeutics; in vitro and in vivo molecular imaging; medicinal inorganic chemistry for infectious disease and cancer applications.

Chiu, Melanie, Ph.D., 2009, University of California, Berkeley: organic, supramolecular, and materials chemistry; synthesis and applications of sequence-defined polymers.

Johnson, Christopher, Ph.D., 2011, University of California, San Diego: Physical Chemistry, Chemical Physics. Molecular spectroscopy; reaction dynamics; characterization of reaction intermediates; atmospheric chemistry; catalysis; mass spectrometry.

#### Research Faculty

Marschilok, Amy C., Ph.D., University at Buffalo (SUNY); Inorganic and materials chemistry; preparation and investigation of novel electrode materials and structures for energy storage, including metal-air batteries.

# **Affiliated Professors**

Knopf, Daniel, Ph.D., 2003, Swiss Federal Institute of Technology: Atmospheric Chemistry. Multiphase chemical kinetics and phase transition of aerosol particles. Classical nucleation theory. Mass spectrometry and surface and micro-spectroscopic analytical techniques. Primary appointment: School of Marine and Atmospheric Sciences

Rizzo, Robert C., Ph.D., 2001, Yale University: Structure-based drug design, computational structural biology, docking, molecular dynamics. Quantifying molecular recognition with quantitative structural biology. Primary appointment: Department of Applied Math and Statistics.

Weinacht, Thomas, Ph.D., 2000, University of Michigan: Time resolved spectroscopy and Strong Field Quantum Control. Primary appointment: Department of Physics and Astronomy.

## Affiliated Associate Professors

Green, David, Ph.D., 2002, Massachusetts Institute of Technology: Computational biology of protein interactions. Primary appointment: Department of Applied Math and Statistics.

Koga, Tadanori, Ph.D., 1998, Kyushu University, Japan: Green polymer nanoprocessing and nanofabrication, structure and dynamics of polymeric nanomaterials using x-ray and neutron scattering, Primary appointment: Department of Materials Science and Chemical Engineering. Primary appointment: Department of Materials Science and Chemical Engineering.

Orlov, Alexander, Ph.D., 2005, University of Cambridge, United Kingdom: Physical and environmental chemistry; materials science and engineering; heterogeneous catalysis; novel materials for environmental and energy applications; environmental engineering and environmental science. Primary appointment: Department of Materials Science and Engineering.

Seeliger, Markus, Ph.D., 2003, Cambridge University: Chemical Biology, biochemistry, structural biology, biophysics. Protein-Drug Interactions. Primary appointment: Department of Pharmacological Sciences.

#### **Affiliated Assistant Professors**

Reuter, Matthew G., Ph.D., 2011, Northwestern University: Nanomaterials, computational chemistry, non-equilibrium dynamics. Quantifying electron dynamics in chemical systems driven from equilibrium. Primary appointment: Department of Applied Math and Statistics, Institute for Advanced Computational Science.

Seeliger, Jessica, Ph.D., 2007, Stanford University: Chemical biology, biochemistry, microbiology. Mechanisms of lipid membrane biogenesis in bacterial pathogens; inhibitor discovery and characterization. Primary appointment: Department of Pharmacological Sciences.

## **Affiliated Adjunct Professors**

Liu, Ping, Ph.D., 1994, Jilin University: Theoretical description of nanostructures, supported nanostructures, surfaces and their catalytic applications in heterogeneous catalysis and electrocatalysis, with a focus on catalytic processes in production, conversion and use of non-conventional fuels such as hydrogen and alcohols. Density functional calculations, kinetic modeling and sensitivity analysis are employed to obtain a fundamental understanding of catalytic processes and provide guidance for the catalyst development. Primary appointment: Brookhaven National Laboratory.

Miller, Lisa, Ph.D., Biophysics, 1995, Albert Einstein College of Medicine: Study of the chemical makeup of tissue in disease, using high-resolution infrared and x-ray imaging at the National Synchrotron Light Source (NSLS). Primary appointment: Brookhaven National Laboratory.

Misewich, James, Ph.D., 1984, Cornell University: Associate Laboratory Director for Basic Energy Sciences, which is responsible for overseeing research in chemistry, condensed matter physics, materials science and nanoscience. Primary appointment: Brookhaven National Laboratory.

Rodriguez, Jose A., Ph.D., 1988, Indiana University: Surface chemistry and catalysis. Primary appointment: Brookhaven National Laboratory.

Shanklin, John, Ph.D.,1988, University of Wisconsin-Madison: Biochemistry of lipid metabolism, enzyme structure-function studies, understanding enzyme specificity, redesigning enzymes for new functionality, understanding biochemical regulation processes, metabolic engineering of plants to accumulate unusual fatty acids and to accumulate oil in vegetative tissues. Primary appointment: Brookhaven National Laboratory.

Stacchiola, Dario, Ph.D., 2002 University of Wisconsin-Milwaukee: Surface chemistry and structure-activity relationships in catalysis. Primary appointment: Brookhaven National Laboratory.

Stavitski, Eli, Ph.D., 2006, Hebrew University of Jerusalem: Operando characterization of advanced functional materials; heterogeneous catalysis; nanoporous frameworks. Primary appointment: Brookhaven National Laboratory.

Zhu, Yimei, Ph.D., 1987, Nagoya University: Nanoscale structure and property relations in oxides, strongly correlated electron systems and energy materials, advanced electron microscopy. Primary appointment: Brookhaven National Laboratory.

Zuckermann, Ronald, Ph.D., 1989, University of California, Berkeley: Solid-phase synthesis of sequence-defined polymers. Design, synthesis and folding of peptoid polymers into protein-mimetic nanostructures, screening of combinatorial libraries for function. Primary appointment: Lawrence Berkeley National Laboratory.

Number of teaching, graduate, and research assistants, fall 2019: 179

- 1) Recipient of the State University Chancellor's Award for Excellence in Teaching, 1990; Recipient of the President's Award for Excellence in Teaching, 1990.
- 2) Joint appointment, Department of Biochemistry.
- 3) Joint appointment, Department of Geosciences. Recipient of the State University Chancellor's Award for Excellence in Scholarship and Creative Activities, 2008.
- 4) Joint appointment, Materials Sciences and Engineering.
- 5) Recipient of the State University Chancellor's Award for Excellence in Teaching, 1986.
- 6) Recipient of the State University Chancellor's Award for Excellence in Scholarship and Creative Activities, 2018.
- 7) Joint appointment, Department of Pharmacology.
- 8) Recipient of the State University Chancellor's Award for Excellence in Teaching, 1998; Recipient of the President's Award for Excellence in Teaching, 1998.
- 9) Joint appointment, Department of Physics & Astronomy.

NOTE: The course descriptions for this program can be found in the corresponding program PDF or at COURSE SEARCH.