CHEMISTRY

Sterling Chemistry Laboratory, 203.432.3913
http://chem.yale.edu
M.S., Ph.D.

Chair
Kurt Zilm (chemistry.chair@yale.edu)

Director of Graduate Studies
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Professors Victor Batista, Gary Brudvig, Robert Crabtree (*Emeritus*), Craig Crews,* R. James Cross, Jr. (*Emeritus*), Jonathan Ellman, John Faller (*Emeritus*), Sharon Hammes-Schiffer, Nilay Hazari, Seth Herzon, Patrick Holland, Mark Johnson, William Jorgensen, J. Patrick Loria, James Mayer, J. Michael McBride (*Emeritus*), Scott Miller, Peter Moore (*Emeritus*), Anna Pyle,* James Rothman,* Martin Saunders, Dieter Söll,* David Spiegel, Scott Strobel,* John Tully (*Emeritus*), Patrick Vaccaro, Elsa Yan, Frederick Ziegler (*Emeritus*), Kurt Zilm

Associate Professors Jason Crawford, Timothy Newhouse

Assistant Professors Caitlin Davis, Ziad Ganim, Stavroula Hatzios,* Sarah Slavoff, Hailiang Wang

Lecturers Paul Anastas, Paul Cooper, Christine DiMeglio, Narasimhan Ganapathi, Jonathan Parr

* A secondary appointment with primary affiliation in another department.

FIELDS OF STUDY

Fields include bio-inorganic chemistry, bio-organic chemistry, biophysical chemistry, chemical biology, chemical physics, inorganic chemistry, materials chemistry, organic chemistry, physical chemistry, physical-inorganic chemistry, physical-organic chemistry, synthetic-organic chemistry, and theoretical chemistry.

SPECIAL REQUIREMENTS FOR THE PH.D. DEGREE

A foreign language is not required. Five term courses are required within the first two years of residence. Courses are chosen according to the student's background and research area. To be admitted to candidacy a student must (1) receive at least two term grades of Honors, exclusive of those for research; (2) pass one oral examination – or, for biophysical chemistry students, two oral examinations – by the end of the second year of study; and (3) submit a thesis prospectus no later than the end of the third year of study. Remaining degree requirements include completing a formal independent proposal by the end of the fourth year, a written thesis describing the research, and an oral defense of the thesis. The ability to communicate scientific knowledge to others outside the specialized area is crucial to any career in chemistry. Therefore, all students are required to teach a minimum of two terms. Students who require additional support from the Graduate School must teach additional terms, if needed, after they have fulfilled the academic teaching requirement. All students are required to take

CHEM 590, Ethical Conduct and Scientific Research, in the fall term of their first year of study.

Ph.D. program materials are available online at https://chem.yale.edu/academics/graduate-program/current-students/forms-steps-phd.

INTEGRATED GRADUATE PROGRAM IN PHYSICAL AND ENGINEERING BIOLOGY (PEB)

Students applying to the Ph.D. program in Chemistry in the biophysical or theoretical subfields may also apply to be part of the PEB program. See the description under Non-Degree-Granting Programs, Councils, and Research Institutes for course requirements, and http://peb.yale.edu for more information about the benefits of this program and application instructions.

MASTER'S DEGREE

M.S. (en route to the Ph.D.) A student must pass at least five graduate-level term courses in the Chemistry department exclusive of seminars and research. In addition, an overall average (exclusive of seminars and research) of High Pass must be maintained in all courses. One full year of residence is required.

COURSES

CHEM 502a, Fundamentals of Transition Metal Chemistry Patrick Holland
This half-term course covers the structures and properties of coordination compounds, and strategies for the design and analysis of new compounds. Elements of chelating ligands, spectroscopic methods, and magnetism are addressed. Prerequisites: two terms of organic chemistry and one term of inorganic chemistry (CHEM 252 or equivalent). ½ Course cr

CHEM 509a, Research Frontiers in Materials Chemistry Hailiang Wang
This course aims to serve graduate and senior undergraduate students from various academic departments who are interested in learning advanced chemistry and nanoscience for performing materials-related research. Material synthesis methods and structure characterization techniques are discussed in detail, with the focus on understanding fundamental structure-property correlations. Special topics on state-of-the-art materials chemistry research are also covered, including graphene and carbon nanotubes, inorganic nanocrystals, catalysis, battery materials, etc. Prerequisites: Undergraduate level general chemistry, inorganic chemistry, and physical chemistry, or equivalent level of knowledge. ½ Course cr

CHEM 514a, Molecular Materials: Design, Synthesis, and Properties Amymarie Bartholomew
Materials synthesized from molecular building blocks have an extraordinary range of properties (porosity, magnetism, conductivity, and combinations thereof, etc.), which depend on the molecular components and the manner in which they are assembled. This course introduces ways to understand and predict the properties of molecularly derived materials from their constituent molecules and their covalent, ionic, or spatial interactions upon assembly. The course also introduces techniques used to synthesize and study molecular materials, with the goal of providing students with a holistic understanding of research in this field. Prerequisite: Fundamentals of Transition Metal Chemistry (CHEM 402) or permission of the instructor. ½ Course cr

CHEM 516a, Organic Structure and Energetics William Jorgensen
The course covers concepts in physical organic chemistry including molecular structure and bonding, conformational energetics, electronic effects, thermochemistry, ring strain, noncovalent interactions, molecular recognition, and host-guest chemistry. Prerequisites: two terms of organic chemistry and two terms of physical chemistry, or related courses, or permission of the instructor. ½ Course cr

CHEM 517a, Kinetics and Thermodynamics in Organic Systems William Jorgensen
The course generally follows CHEM 516. This module covers concepts in physical organic chemistry including acid-base chemistry, advanced issues in stereochemistry, kinetics, and thermodynamics, as well as experiments and techniques employed in mechanistic analysis. Issues in catalysis are addressed throughout. Prerequisites: CHEM 516, two terms of introductory organic chemistry, and two terms of physical chemistry. Permission of the instructor may be sought for potential exceptions. ½ Course cr

CHEM 519a, Foundations of Chemical Biology Jason Crawford
Chemical biology is a rapidly developing field at the interface of chemical and biological sciences. This subject deals with how chemistry can be applied to manipulate and study biological problems using a combination of experimental techniques ranging from organic chemistry to analytical chemistry, biochemistry, molecular biology, biophysical chemistry, and cell biology. The purpose of this course is to teach students the core skills that are used by scientists at the interface of chemistry and biology. The course transitions into CHEM 522, where students learn more about therapeutic applications of chemical biology. Prerequisites: two terms of both general chemistry and organic chemistry. ½ Course cr

CHEM 529a, Total Synthesis Timothy Newhouse
This course is conducted as a seminar. The content focuses on modern strategies and tactics in natural product synthesis with a focus on alkaloids, terpenes, and polyketides. One objective of the course is to introduce strategy level decision making considering multiple approaches to retrosynthetic disconnection. Additionally, a wide variety of methodologies are described and discussed with respect to how they can be implemented in total synthesis. The course draws from primary sources in order for students to develop critical reading and writing skills. Prerequisite: one chemistry course at the 500 level or permission of the instructor. ½ Course cr

CHEM 532a, Synthetic Methods in Organic Chemistry I Jon Ellman
Compound synthesis is essential to the discovery and development of new chemical entities with a desired property, whether for fundamental study or a more applied goal such as a new pharmaceutical, agrochemical, or material. In this course we emphasize key transformations and principles to provide a framework for the efficient design and synthesis of organic compounds. Prerequisites: two terms of organic chemistry and one term of introductory inorganic chemistry, or related course, or permission of the instructor. ½ Course cr

CHEM 533a, Synthetic Methods in Organic Chemistry II Timothy Newhouse
Compound synthesis is essential to the discovery and development of new chemical entities with a desired property, whether that be for fundamental study or for a more applied goal such as a new pharmaceutical, agrochemical, or material. In this course we emphasize key transformations and principles to provide a framework for the efficient

design and synthesis of organic compounds. This course builds on the knowledge learned in CHEM 532. Prerequisite: CHEM 532 or permission of the instructor. ½ Course cr

CHEM 566a, Introduction to Quantum Mechanics I Sharon Hammes-Schiffer
An introduction to quantum mechanics, starting with the Schrödinger equation and covering model systems such as particle-in-a-box and harmonic oscillator. The fundamental postulates and theorems of quantum mechanics are also covered. Prerequisite: physical chemistry, multivariable calculus or equivalent experience, or permission of the instructor. ½ Course cr

CHEM 567a, Introduction to Quantum Mechanics II Sharon Hammes-Schiffer
Continuation of an introduction to quantum mechanics, starting with angular momentum and the hydrogen atom, and then covering approximate methods such as the variation method and perturbation theory. The concepts of electron spin as well as Hartree-Fock theory and other electronic structure methods for describing molecules are also covered. Prerequisite: CHEM 566, multivariable calculus, or equivalent experience. ½ Course cr

CHEM 572a, Introduction to Statistical Mechanics I Victor Batista
An introduction to modern statistical mechanics, starting with fundamental concepts of quantum statistical mechanics to establish a microscopic derivation of statistical thermodynamics. Topics include ensembles; Fermi, Bose, and Boltzmann statistics; density matrices; mean-field theories; phase transitions; chemical reaction dynamics; time-correlation functions; Monte Carlo simulations; and molecular dynamics simulations. Prerequisite: physical chemistry, multivariable calculus, or equivalent experience. ½ Course cr

CHEM 573a, Introduction to Statistical Mechanics II Victor Batista
An introduction to modern statistical mechanics, starting with fundamental concepts of quantum statistical mechanics to establish a microscopic derivation of statistical thermodynamics. Topics include ensembles; Fermi, Bose, and Boltzmann statistics; density matrices; mean-field theories; phase transitions; chemical reaction dynamics; time-correlation functions; Monte Carlo simulations; and molecular dynamics simulations. Prerequisite: physical chemistry, multivariable calculus, or equivalent experience. ½ Course cr

CHEM 574a, Experimental Physical Methods in Molecular Sciences I Caitlin Davis
Applications of modern experimental physical methods to molecular science. Emphasis is placed on interpreting experimental data obtained by various physical methods to gain structural and dynamic information to solve problems at the molecular level. A wide range of methods are covered, such as nonlinear spectroscopy, optical imaging, vibrational spectroscopy, NMR, and electrochemical methods. Discussions focus on current and classic literature in the fields. Prerequisite: Undergraduate physical chemistry, or permission of instructor. Students enrolled in Chem 574 are expected to also enroll in Chem 575. ½ Course cr

CHEM 575a, Experimental Physical Methods in Molecular Sciences II Caitlin Davis
Applications of modern experimental physical methods to molecular science. Emphasis is placed on interpreting experimental data obtained by various physical methods to gain structural and dynamic information to solve problems at the molecular level. A wide range of methods is covered, such as nonlinear spectroscopy, optical imaging,

vibrational spectroscopy, NMR, and electrochemical methods. Discussions focus on current and classic literature in the fields. This class is the second half of Chem 574, which is a prerequisite. It is expected that Chem 574 & Chem 575 will be taken in the same semester, with Chem 574 taught in the first half of the semester and Chem 575 taught in the second half of the semester. ½ Course cr

CHEM 578a, Molecules and Radiation I: Matrix Methods in Quantum Mechanics Patrick Vaccaro
A treatment of time-independent quantum mechanics especially aimed at applications in spectroscopy focusing on the use of matrix methods. Development of basis sets, time-independent perturbation theory, matrix mechanics, angular momentum, and basic group theory. Prerequisite: previous exposure to quantum mechanics at the level of physical chemistry, or permission of the instructor. ½ Course cr

CHEM 585a, Protein NMR Spectroscopy J Patrick Loria
A theoretical treatment of solution NMR spectroscopy with emphasis on applications to proteins and biological macromolecules. This includes classical and quantum mechanical descriptions of NMR, product operator formalism, multidimensional NMR, phase cycling, gradient selection, relaxation phenomena, and protein resonance assignments. Prerequisite: physical chemistry that includes quantum mechanics; calculus and linear algebra are recommended but not required. ½ Course cr

CHEM 590a, Ethical Conduct and Scientific Research Jonathan Parr
A survey of ethical questions relevant to the conduct of research in the sciences with particular emphasis on chemistry. A variety of issues, including plagiarism, the falsification of data, and financial malfeasance, are discussed, using as examples recent cases of misconduct by scientists. Enrollment is restricted to graduate students in chemistry. 0 Course cr

CHEM 600a, Research Seminar Staff
Presentation of a student's research results to the student's adviser and fellow research group members. Extensive discussion and literature review are normally a part of the series.

CHEM 720a, Current Topics in Organic Chemistry Jon Ellman
A seminar series based on invited speakers in the general area of organic chemistry.

CHEM 730a, Theoretical Chemistry Seminar Kurt Zilm
A seminar series based on invited speakers in the areas of theoretical chemistry.

CHEM 740a, Seminar in Chemical Biology Jon Ellman

CHEM 750a, Biophysical and Physical Chemistry Seminar J Patrick Loria
A seminar series based on invited speakers in the areas of biophysical and physical chemistry.

CHEM 760a, Seminar in Inorganic Chemistry Nilay Hazari

CHEM 980a, Introduction to Research for Long Rotations Staff
During the fall term, first year chemistry graduate students in long rotations are introduced to research during their first laboratory rotation. At the end of the first rotation, students in the course present an oral presentation on their research. The presentation is no longer than ten minutes with a question-and-answer period of no

longer than five minutes. Enrollment requires that a student be a first-year graduate student participating in long rotations.

CHEM 990a, Research Staff
Individual research for Ph.D. degree candidates in the Department of Chemistry, under the direct supervision of one or more faculty members.