CHEMISTRY

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

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

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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 503a, Fundamentals of Organometallic Chemistry  Patrick Holland
A half-term survey of the main principles of organometallic chemistry that enables students to understand basic concepts in the field. It prepares students for CHEM 504, the second half of this course. Prerequisites: two terms of organic chemistry and one term of inorganic chemistry (CHEM 252) or equivalent experience. ½ Course cr

CHEM 504b, Applications of Organometallic Chemistry  Nilay Hazari
A half-term survey of the applications of organometallic chemistry demonstrating the range of areas where organometallic reactions are important. It builds on the knowledge learned in CHEM 503. Prerequisite: CHEM 503 or equivalent experience. ½ Course cr

CHEM 505b, Inorganic Reaction Mechanisms  James Mayer
This half-term course covers the fundamentals of kinetics and mechanisms used by coordination compounds and transition-metal catalysts, and features analysis of papers from the recent literature. Prerequisites: two terms of organic chemistry, one term of inorganic chemistry, and CHEM 502 or equivalent. ½ Course cr

CHEM 506b, Bioinorganic Spectroscopy  Gary Brudvig
This course is an advanced introduction to biological inorganic chemistry with an emphasis on the methods used to characterize the active sites of metalloproteins. The major physical methods used in the determination of molecular structure, bonding, and physical properties of metal ions in proteins are introduced. Prerequisite: a general
Chemistry

knowledge of biochemistry and familiarity with both inorganic coordination chemistry and physical chemistry. ½ Course cr

**CHEM 507b, Bioinorganic Mechanisms**  Gary Brudvig
This course is an advanced introduction to biological inorganic chemistry. An overview of the relevant geometric and electronic structures of metalloprotein active sites is presented and related to each protein’s function. The objective is to define and understand the function of metals in biology in terms of structure. Prerequisite: CHEM 506 or permission of the instructor. It is assumed that students have a general knowledge of biochemistry and are familiar with both inorganic coordination chemistry and physical chemistry. 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 511b, Fundamentals of Diffraction for Small Molecule Crystallography**  Brandon Mercado
In the field of chemistry, determining the connectivity of atoms in unknown compounds is critical. Accurate and precise structure models help us understand the function of materials. Single crystal diffraction is an elegant method to determine molecular structure and its related parameters. This course introduces the fundamental concepts of diffraction with a summary of symmetry elements, space group theory, and solving “the phase problem.” The course is designed to provide the foundation for students to critically evaluate not only their own structure models determined by diffraction, but also those presented in the literature and diffraction databases. Prerequisite: inorganic chemistry, CHEM 502, or permission of the instructor. ½ Course cr

**CHEM 512b, The Refinement of Small Molecule Crystal Structures**  Brandon Mercado
In the field of chemistry, determining the connectivity of atoms in unknown compounds is critical. Accurate and precise structure models help us understand the function of materials. Single crystal diffraction is an elegant method to determine molecular structure and its related parameters. This course introduces the practical concepts of how to model a structure from diffraction data. Some of the topics covered include visualizing electron density in a crystal, molecular disorder, twinning, and publication of results. Prerequisite: CHEM 511 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**  Scott Miller
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**  Stacy Malaker
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 520a, Foundations of Chemical Biology II: Protein Design & Catalysis**  Jason Crawford
The lecture component of this course largely focuses on protein function and catalysis of diverse small molecule natural products. The course also serves to teach students on how to write an effective NSF style research proposal in Chemical Biology and communicate its contents to a diverse scientific audience. Prerequisite: CHEM 519 or permission of the instructor. ½ Course cr

**CHEM 524a, Foundations of Chemical Biology II: Applications of Chemical Biology to Therapeutics**  David Spiegel
This course explores the design and enablement of medicines derived from a convergence of concepts and techniques from chemistry and biology. Topics include small-molecule drug discovery concepts and tools, drug metabolism, protein therapeutics, hybrid chemical/biologic drugs, and bifunctional molecules. Modern approaches for target discovery and validation are also discussed. Prerequisite: CHEM 519, two terms of undergraduate organic chemistry, or permission of the instructor. A basic understanding of biochemistry and molecular biology is assumed. ½ Course cr

**CHEM 528b, Natural Products Synthesis**  Seth Herzon
Survey of natural products syntheses, with an emphasis on those that contain unique strategies, transformations, or reagents. Key transformations are introduced in the context of various syntheses. Retrosynthetic analysis and synthetic planning are discussed. Prerequisites: undergraduate organic chemistry and one term of a graduate course in organic chemistry, 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  Jon Ellman
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 535b, Fundamental Medicinal Chemistry  William Jorgensen
The course covers basic concepts of medicinal chemistry including drug structures, properties of drugs, methods of drug discovery, protein-ligand interactions, enzyme inhibition, assays, drug targets, anti-infective agents, virtual and high-throughput screening, structures to avoid (PAINS), structure-based drug design, and metabolism. Prerequisites: undergraduate organic and physical chemistry, or permission of the instructor. ½ Course cr

CHEM 536b, Computer Simulations of Organic and Biomolecular Systems  William Jorgensen
The course covers methods and applications of statistical mechanics and molecular dynamics to model fluid systems including biomolecules in aqueous solution. Topics covered include force fields, Monte Carlo and molecular dynamics theory, simulation of water and other liquids, free-energy methods and applications, QM/MM simulations, protein dynamics, and molecular recognition and design. Prerequisites: undergraduate organic and physical chemistry, or permission of the instructor. ½ Course cr

CHEM 560La, Advanced Instrumentation Laboratory I  Patrick Vaccaro
A laboratory course introducing physical chemistry tools used in the experimental and theoretical investigation of large and small molecules. Modules include electronics, vacuum technology, optical spectroscopy and lasers, and computer programming. 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 E. Chui-Ying Yan
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 E. Chui-Ying Yan
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 576a, Fundamentals for Physical Chemistry Mark Johnson
This course reinforces the principles of physics that are most relevant to experimental and theoretical physical chemistry. These include classical electricity and magnetism (with emphasis on the nature of light and the interaction of light with matter), optics, lasers, angular momentum, and atomic structure, including the spin-orbit interaction. The basic theme of the course is to provide students with physical intuition that can bridge the observations of everyday experience to the abstract concepts required for the correct, quantum-mechanical description of atomic-scale phenomena. Prerequisites: two terms of undergraduate physical chemistry (CHEM 328 or CHEM 332, and
CHEM 333; or equivalents); and physics course work covering classical mechanics and electrostatics. ½ Course cr

CHEM 578a, Molecules and Radiation I: Matrix Methods in Quantum Mechanics
Kurt Zilm
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 579a, Molecules and Radiation II: Time-Dependent Quantum Mechanics and Spectroscopy
Kurt Zilm
A treatment of time-dependent quantum mechanics especially aimed at applications in spectroscopy. Sudden and adiabatic processes, interaction of radiation with electric and magnetic dipoles, Fermi’s golden rule, two-level systems and Rabi cycling, spontaneous emission and relaxation kinetics, Bloch equations, line shapes and relaxation theory, illustrations chosen from optical and magnetic resonance. Prerequisite: CHEM 578 or permission of the instructor. ½ Course cr

CHEM 584b, Machine Learning and Quantum Computing in Chemistry and Materials Science
Victor Batista
Machine learning and quantum computing have emerged as leading technologies of the twenty-first century and are expected to be increasingly applied to a wide variety of chemical and materials science challenges. This course introduces fundamental concepts of machine learning and quantum computing to chemists and materials science students through an overview of algorithms, computational methods, and applications. It is intended to empower students to engage with this emerging field and foster the growing field of artificial intelligence for accelerated scientific discoveries in the molecular and physical sciences. Prerequisites: introductory quantum mechanics and Python, or permission of the instructor. ½ Course cr

CHEM 588b, Optical Spectroscopy: Applications in Biophysics
E. Chui-Ying Yan
The course covers basic theory of fluorescence and vibrational spectroscopies and their applications in biophysics. Emphasis is placed on quantitative interpretation of experimental data to gain structural and dynamic information to address biological questions at the molecular level. Topics include fluorescence correlation spectroscopy (FCS); Forster resonance energy transfer (FRET); fluorescence anisotropy; and Raman, infrared, and non-linear optical spectroscopies. Discussions of applications focus on current and classic literature. This course provides foundational knowledge for advanced courses on molecular optical imaging. Prerequisite: undergraduate upper-level physical chemistry or permission of the instructor. ½ Course cr

CHEM 590a, Ethical Conduct and Scientific Research
E. Chui-Ying Yan
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 592b, Biochemical Rates and Mechanisms I  J Patrick Loria  
An advanced treatment of enzymology. Topics include transition state theory and derivation of steady-state and pre-steady-state rate equations. The role of entropy and enthalpy in accelerating chemical reactions is considered, along with modern methods for the study of enzyme chemistry. These topics are supplemented with in-depth analysis of the primary literature. Prerequisites: CHEM 332 or equivalent, two terms of organic chemistry, and MATH 115.  ½ Course cr

CHEM 593b, Biochemical Rates and Mechanisms II  J Patrick Loria  
This course focuses on the role of molecular motions in enzyme function, and on biochemical and spectroscopic methods to interrogate these motions. Examples explore motions ranging from picoseconds to milliseconds and how the timescales and amplitudes of these motions impact catalysis and allostery. Prerequisite: CHEM 592 or permission of the instructor.  ½ Course cr

CHEM 596b, Computational Chemistry  Sharon Hammes-Schiffer  
An introduction to modern computational quantum chemistry methods. The lectures cover Hartree-Fock theory, density functional theory, geometry optimizations, thermochemistry, transition states, minimum energy paths, continuum solvation models, electron correlation methods, and modeling excited states. Special emphasis on the hands-on use of computational packages for current applications spanning organic, inorganic, and biochemical reactions. Prerequisite: physical chemistry or permission of the instructor.  ½ Course cr

CHEM 600a or b, 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 and CHEM 721b, Current Topics in Organic Chemistry  Staff  
A seminar series based on invited speakers in the general area of organic chemistry.

CHEM 730a and CHEM 731b, Theoretical Chemistry Seminar  Staff  
A seminar series based on invited speakers in the areas of theoretical chemistry.

CHEM 740a and CHEM 741b, Seminar in Chemical Biology  Staff  
A seminar series based on invited speakers in the areas of biophysical and physical chemistry.

CHEM 760a and CHEM 761b, Seminar in Inorganic Chemistry  Staff  
A seminar series based on invited speakers in the general area of inorganic chemistry.
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 graduate student who has participated in short rotations.

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