CHEMISTRY

Sterling Chemistry Laboratory, 203.432.3915
http://chem.yale.edu
M.S., Ph.D.

Chair
Nilay Hazari (chemistry.chair@yale.edu)

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

Associate Professors Stavroula Hatzios,* Sarah Slavoff

Assistant Professors Amymarie Bartholomew, Caitlin Davis, Stacy Malaker, Mingjiang Zhong,* Tianyu Zhu.

Lecturers Paul Anastas,* Paul Cooper, Christine DiMeglio, Laura Herder, Jonathan Parr.

* A secondary appointment with primary affiliation in another department.

FIELDS OF STUDY

Fields include biophysical chemistry, chemical biology, inorganic chemistry, materials chemistry, organic chemistry, physical 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 and (2) pass the candidacy exam by the end of the second 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.

MASTER'S DEGREE

M.S. (en route to the Ph.D.) A student must pass at least five graduate-level term courses in the Department of Chemistry, 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 503b, Fundamentals of Organometallic Chemistry Nilay Hazari
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 James Mayer
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 506a, 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 knowledge of biochemistry and familiarity with both inorganic coordination chemistry and physical chemistry. ½ Course cr

CHEM 507a, 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 510a, Energy and Environmental Electrochemistry Hailiang Wang
This course aims to serve graduate and senior undergraduate students from various academic departments who are interested in learning electrochemistry and its related materials chemistry for performing energy and environmental research. The most important task of this course is to discuss and understand how the properties of electrochemical energy storage and conversion devices are fundamentally determined by their chemistry. Battery and electrocatalytic reactions that are of current research focus are introduced and discussed in detail. State-of-the-art materials development, structural characterization, electrochemical reaction studies, mechanistic investigation, and reactor engineering related to these reactions are also be covered. Prerequisites: undergraduate-level general chemistry (CHEM 161 and CHEM 165 *or* CHEM 163 and CHEM 167), inorganic chemistry (CHEM 252), and thermodynamics/physical chemistry (CHEM 332) or equivalent level of knowledge. ½ Course cr

CHEM 513a, Electronic Structure in Inorganic Chemistry Patrick Holland
This course covers a number of methods for analyzing the electronic structure of coordination complexes of the transition metals. It features the use of density-functional theory (DFT) to gain quantitative insight into properties, and critical analysis of the results. Prerequisite: CHEM 502 or equivalent. 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, Proteomics and Chemical Glycobiology Stacy Malaker
Chemical biology deals with how chemistry can be applied to manipulate and study biological problems using techniques from organic chemistry, analytical chemistry, biochemistry, molecular biology, biophysical chemistry, and cell biology. This course covers topics related to the structure of proteins and oligosaccharides, protein engineering and labeling, and glycosylated proteins/nucleic acids. These play important roles throughout biochemistry and human health. Prerequisites: two terms of organic chemistry. ½ Course cr

CHEM 521a, Protein Design and Catalysis Jason Crawford
The lecture component of this course largely focuses on protein function, catalysis, and the chemistry and biology of diverse small molecule products. The course also serves to support students in writing an effective NSF style research proposal in chemical biology and communicating its contents to a diverse scientific audience. Prerequisites: Two semesters of undergraduate organic chemistry (CHEM 174/175 and/or CHEM

220/221). A basic understanding of biochemistry and molecular biology is also assumed, but you can "catch up" by carefully and thoroughly reading the course materials and recommended books. ½ Course cr

CHEM 524a, Chemical Biology of Drug Discovery 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 bi-functional molecules. Modern approaches for target discovery and validation are also discussed. The course is not organized around a textbook. Rather, material covered in lectures is the focus of the course and supplementary reading is recommended, mostly from modern research literature. Reading lists are distributed at the outset of the module. Prerequisites: two terms of undergraduate organic chemistry, biochemistry, and molecular biology. ½ Course cr

CHEM 529b, 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 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 534b, Synthetic Methods in Drug Discovery and Development Jon Ellman
Synthetic methods that see extensive use in drug discovery and development but are not typically covered in undergraduate- or graduate-level courses are explored. We analyze common structural motifs in drugs and reactions for their preparation. Topics include common methods for the synthesis of amines, catalytic and non-catalytic methods for the formation of aromatic and heteroaromatic C-N and C-O bonds, properties of heterocycles and methods for their elaboration, annulations to common

five- and six-membered heterocycles, and key attributes of the fluorine substituent in drugs along with practical methods for its introduction. Prerequisites: CHEM 532 and CHEM 533, 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 565La, Introduction to Glass Blowing Patrick Vaccaro
This course provides a basic introduction to the fabrication of scientific apparatus from glass. Topics covered include laboratory set-up, the fundamental skills and techniques of glassblowing, the operation of glass fabrication equipment, and requisite safety procedures. Emphasis is placed on manipulative skills and dexterity, as well as the basic tools, materials, and equipment found in a modern glassblowing facility. Students learn through formal and informal lectures, supplemented by extensive hands-on training in the methods of glass heating and manipulation. All students must have permission of their advisor to enroll. Class is limited to five students. All class material is provided; students only need to be on time and wear proper laboratory attire. Please feel free to contact the instructor, Daryl Smith (daryl.smith@yale.edu), if you have any questions or to check availability. A word of advice: the course is more satisfying if you put in extra time outside of the normal course time for practice. ½ Course cr

CHEM 566a, Introduction to Quantum Mechanics I Tianyu Zhu
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 Tianyu Zhu
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 Mark Johnson
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 576b, 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 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 586a, Quantitative Biochemical Imaging Caitlin Davis
Theory of optical microscopy, imaging, and image analysis with emphasis on quantitative characterization of the structure, dynamics, and chemical reactions of proteins, nucleic acids, and other biopolymers. Topics include optics of microscope and image formation, interaction of light and matter, fluorescent probes and biosensors, digital image processing, modern approaches in light microscopy (including confocal and multiphoton), and a brief introduction to electron microscopy and scanning probe techniques. Prerequisite: physical chemistry that includes quantum mechanics; calculus and linear algebra are recommended but not required. 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 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 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 594b, Resonant and Non-Resonant Interaction of Light with Matter Mark Johnson
This course considers the interaction of light with individual molecules and collections of molecules in solutions and solids from the perspective of a classical radiation field interacting with the energy levels that arise from quantized motions. We begin with the generation of light by accelerated charges as described by Maxwell's equations for the electric and magnetic fields. We then consider the polarization states of light, how the oscillating electric field drives the motions of electrons, and how this results in scattering when off-resonant and then evolves into shifts in level populations as the frequency approaches that of the eigenenergies between levels. Classical analogies to quantum mechanical behavior are stressed in the context of the damped-driven electron in a harmonic potential (the so-called Drude model). The kinetics of absorption and emission are discussed in the context of the Einstein treatment that leads to light amplification and laser action. Finally, we develop the "selection rules" that describe what transitions can occur depending on the light polarization and the character of the electronic and nuclear motions. Prerequisite: an upper-level undergraduate physics course in electricity and magnetism or CHEM 576. ½ Course cr

CHEM 596b, Computational Chemistry William Jorgensen
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, 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 Jon Ellman
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 Jon Ellman

CHEM 750a and CHEM 751b, 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 and CHEM 761b, Seminar in Inorganic Chemistry Patrick Holland

CHEM 980a and CHEM 981b, 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 984b, Introduction to Research for Short Rotations Staff
First-year chemistry graduate students with short rotations have joined labs by the end of the fall term. During the spring term, each student is introduced to research by their dissertation research advisors. Towards the end of the spring term, 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 graduate student who has participated in short 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.