

CHEMISTRY (CHM)

Master of Science, Doctor of Philosophy Overview

The Department of Chemistry offers programs of study leading to the MS and PhD degrees. Opportunities for study in courses and through research are available in analytical, biological, inorganic, organic, and physical chemistry. Research plays a major role in the graduate program. Since the number of graduate students is limited, the research program of the individual student is enhanced by close daily contact with the faculty.

All applicants for graduate work in the department are expected to offer as preparation college level fundamental courses in general, analytical, organic, inorganic, and physical chemistry; physics; and mathematics through one year of calculus. During registration all new graduate students take qualifier examinations covering the fields of analytical, biological, inorganic, organic, and physical chemistry. Programs of study are in part determined by the results of these examinations, and deficiencies are to be remedied during the student's first academic year.

For the MS degree, the student is expected to undertake a broad program of coursework at an advanced level and to complete successfully an original investigation. This investigation must be of the highest quality but necessarily limited in scope. Students who hold assistantships typically spend two years in residence for the completion of this degree.

For the PhD degree, individual programs are designed for each student under the guidance of the student's faculty adviser and advisory committee and with the approval of the graduate committee.

The University preliminary examination requirement is satisfied by successful completion of a series of written cumulative examinations and by presentation of two research proposals, one of which is the dissertation research project. Each student is to present at least one departmental seminar on the results of his or her dissertation research. The student must present a dissertation and pass an examination on it as prescribed by the Graduate School, and other University requirements must be satisfied.

The chemistry program participates in the Interdisciplinary Graduate Track in Structural and Computational Biophysics. For more information, refer to the pages in this bulletin regarding the program.

The original graduate program, which led to the MS degree, was discontinued in 1949. The present MS program was begun in 1961, the PhD in 1972.

Graduate courses offered by the Department of Chemistry are from the following list. Not all courses are offered every year.

Programs

- Chemistry, MS (<https://bulletin.wfu.edu/graduate/programs/degree-programs/chemistry/chemistry-ms/>)
- Chemistry, PhD (<https://bulletin.wfu.edu/graduate/programs/degree-programs/chemistry/chemistry-phd/>)
- MD/PhD (<https://bulletin.wfu.edu/graduate/programs/dual-degrees/md-phd/>)
- PhD/MBA (<https://bulletin.wfu.edu/graduate/programs/dual-degrees/phd-mba/>)

- Structural and Computational Biophysics (SCB), Certificate (<https://bulletin.wfu.edu/graduate/programs/certificates/structural-computational-biophysics-scb-certificate/>)

Courses

CHM 621. Intermediate Organic Chemistry. (3 h)

Survey of advanced topics in organic chemistry including stereochemistry, conformational analysis, reaction mechanisms, organometallic chemistry and asymmetric synthesis.

CHM 623. Organic Analysis. (4 h)

The systematic identification of organic compounds.

CHM 624. Medicinal Chemistry. (3 h)

This course is an introduction to drug targets, mechanism, design, and synthesis. Topics of study include the review of biomolecular structure and function; druggable/targetable enzymes and signaling networks; the replisome- and transcriptome as targets; molecular and cellular pharmacology, molecular mechanism of action at the target level; drug metabolism and pharmacokinetics/pharmacodynamics. A significant portion of the course will be devoted to drug discovery, which includes design, SAR, optimization, synthetic methodologies, computer-assisted drug design; QSAR; prodrugs and "bench-to-bedside", approaches.

CHM 625. Organic Synthesis. (4 h)

Reagents for and design of synthetic routes to organic molecules.

CHM 626. Organic Synthesis. (4 h)

Reagents for and design of synthetic routes to organic molecules.

CHM 634. Chemical Analysis. (3, 4 h)

Theoretical and practical applications of modern methods of chemical analysis. C-CHM 641.

CHM 641. Physical Chemistry. (3, 4 h)

Fundamentals of physical chemistry.

CHM 642. Physical Chemistry. (3, 4 h)

Fundamentals of physical chemistry.

CHM 644. Physical Chemistry. (3, 4 h)

Fundamentals of physical chemistry.

CHM 648. Electronic Structure Theory and Computational Chemistry. (3 h)

Introduction to quantum mechanical foundation of electronic structure theory and its application to problems in computational chemistry.

CHM 651. Special Topics in Biochemistry. (3 h)

Fundamentals of biochemistry, with particular emphasis on mechanistic analysis of metabolic pathways, enzymatic activity, and drug action.

CHM 656. Chemical Spectroscopy. (1.5 h)

Fundamental aspects of the theory and application of chemical spectroscopy, as found in the areas of analytical, inorganic, organic, and physical chemistry. Emphasis varies. Seven week courses. P-CHM 642 or 644, 661 or POI. May be repeated for credit.

CHM 657. Chemical Spectroscopy. (1.5 h)

Fundamental aspects of the theory and application of chemical spectroscopy, as found in the areas of analytical, inorganic, organic, and physical chemistry. Emphasis varies. Seven week courses. P-CHM 642 or 644, 661 or POI. May be repeated for credit.

CHM 661. Inorganic Chemistry. (3, 4 h)

Principles and reactions of inorganic chemistry. C-CHM 641.

CHM 662. Nanochemistry in Energy and Medicine. (3 h)

New optoelectronic science and technologies, often involving nanotechnologies, photochemistry, and laser are revolutionizing many fields for solar energy conversion has inspired many researchers across different chemical, physical and engineering disciplines. Implementation of new laser-based optical techniques, photochemistry, and nanotechnology concepts have enabled dramatic progress in biomedical science where their potential is still developing rapidly. The goal of this course is to familiarize students with advanced topics in nanomaterials science, nanosynthesis, photochemistry, energy conversion, optoelectronics, and biomedical photonics. In this course nanomaterials structures, nanodevices, and time-resolved (fs-ms) photochemical processes involved in energy conversion and biomedical applications will be discussed. The energy and optoelectronic materials sections cover a broad range of different systems including organic, inorganic molecular materials, polymers, and semiconductors, applied in energy conversion and optoelectronics. The photochemical processes in these optoelectronic systems will be described. This includes light-driven optical, electronic, and chemical processes in a broad range of materials such as organic molecular materials, metal-organic dyes, polymers and semiconductors, that govern the behavior of optoelectronic and photovoltaic devices. Practical applications, device schemes, different generations, and recent progress in the field will be overviewed. The use of ultrafast laser techniques for the photochemical understanding of optoelectronic materials and interfaces will be covered. The application of nanomaterials and laser spectroscopy techniques in biomedical imaging (biomedical photonics) will be discussed. This includes nanodevices such as biosensors, drug delivery/release systems, for biomedical applications. The laser biomedical imaging techniques and optoelectronic approaches for clinically monitoring of early disease states and molecular diagnostics will be discussed.

CHM 664. Materials Chemistry. (3 h)

A survey of inorganic-, organic-, bio-, and nano-materials, including hybrid materials and applications.

CHM 664L. Materials Chemistry Lab. (1 h)

Synthesis of inorganic and organic based materials and their characterization. Lab-four hours.

CHM 666. Chemistry and Physics of Solid State Materials. (3 h)

Design, synthesis, structure, chemical and physical properties, and the application of solid state materials.

CHM 670. Biochemistry: Macromolecules and Metabolism. (3 h)

A lecture course introducing the principles of biochemistry, with emphasis on the experimental approaches that elucidated these principles. Major topics include structure, function, and biosynthesis of biological molecules, analysis of enzyme function and activity, bioenergetics, and regulation of metabolic pathways.

CHM 673. Biochemistry Protein and Nucleic Acid Structure and Function. (3 h)

Special topics in biochemistry including catalytic mechanisms of enzymes and ribozymes, use of sequence and structure databases, and molecular basis of disease and drug action. P-CHM 670 or POI.

CHM 676. Biophysical Chemistry. (3 h)

Introduction to a variety of technologies (e.g. thermochemistry, electrochemistry, spectrometry, and spectroscopy) for determining physical properties of biomolecules. From these properties, the biological function can be more readily understood and leveraged for medical gain. In addition to problem sets, students will have opportunities to hone science communication skills through a writing assignment and oral presentation. P-CHM 670 or POI.

CHM 681. Chemistry Seminar & Literature. (0.5 h)

Discussions of contemporary research and introduction to the chemical literature and acquisition of chemical information. May be repeated for credit. Pass/Fail only.

CHM 682. Chemistry Seminar & Literature. (0.5 h)

Discussions of contemporary research and introduction to the chemical literature and acquisition of chemical information. May be repeated for credit. Pass/Fail only.

CHM 701. Advanced Physical Chemistry. (3 h)

An accelerated survey of classical and statistical thermodynamics, chemical kinetics, and quantum chemistry. Staff.

CHM 711. Directed Study in Chemistry. (1, 2 h)

Reading and/or lab problems carried out under supervision of a faculty member. P-Permission of graduate committee. May be repeated for credit if topic varies.

CHM 712. Directed Study in Chemistry. (1, 2 h)

Reading and/or lab problems carried out under supervision of a faculty member. P-Permission of graduate committee. May be repeated for credit if topic varies.

CHM 721. Advanced Organic Chemistry. (3 h)

An accelerated survey of organic reactions and mechanisms. King, Welker, Jones.

CHM 722. Physical Organic Chemistry. (3 h)

Physical methods for determining structure-activity correlations and reaction.

CHM 723. Transition-Metal Organic Chemistry. (3 h)

Introduction to principles of bonding in organometallic chemistry and organometallic reaction mechanisms. Uses of transition-metal complexes in organic synthesis. Welker.

CHM 724. Organic Synthesis. (3 h)

Modern principles of organic synthesis and retrosynthetic analysis. Stereoselective synthesis of complex natural products. King, Welker, Jones.

CHM 725. Structure Identification in Organic Chemistry. (3 h)

Theory and use of spectroscopic techniques for structural identification of organic compounds. King, Welker.

CHM 726. Reactive Intermediates. (3 h)

Mechanistic and preparative photochemistry. Structure and chemistry of excited states, free radicals, carbenes, and selected ions. Jones.

CHM 735. Spectrochemical Analysis. (3 h)

Principles of atomic and molecular spectrometric methods; discussion of instrumentation, methodology, and applications.

CHM 736. Chemical Separations. (3 h)

Theory and practice of modern separation methods with emphasis on gas and liquid chromatographic techniques. Hinze, Jones, Colyer.

CHM 737. Electrochemical Processes. (3 h)

Principles of electrochemical methods, ionic solutions, and electrochemical kinetics. Colyer, Hinze, Jones, Nofhle.

CHM 738. Statistics for Analytical Chemistry. (3 h)

Practical investigation of the statistical procedures employed in modern analytical chemistry.

CHM 739. Special Topics in Analytical Chemistry. (3 h)

The study of topical fields of research in analytical chemistry, with a focus on one or more specialities, such as ICP-MS; fluorescence, LIBS; Raman spectroscopy; nanoparticles in analysis; biosensors; or others. May be repeated for credit if course content differs.

CHM 740. Drug Discovery, Design, and Development - Molecules to Medicines. (3 h)

Conducted as a combination of lectures, reading assignments, and student-led discussions. Examines drug discovery and development pathways from target and lead compound identification through metabolic and toxicology studies, clinical trials, FDA approval, and marketing. Regulatory processes, intellectual property, and ethical issues are also considered. Taught by WFU faculty from both the Reynolda and Bowman Gray campuses and colleagues in the pharmaceutical and biotechnology industries, students work in teams to present case studies on the discovery, development, and marketing of recently approved pharmaceuticals. Also listed as BAMB 740. P-Organic chemistry and biochemistry.

CHM 745. Statistical Thermodynamics. (3 h)

The application of statistical mechanics to chemistry to understand and predict the thermodynamic properties. Kondepudi.

CHM 746. Chemical Kinetics. (3 h)

Kinetics and mechanisms of chemical reactions; theories of reaction rates. Swofford, Kondepudi.

CHM 747. Self-Organization in Nonequilibrium Chemistry. (3 h)

Study of the phenomena of self-organization, such as oscillations, multistability, propagating waves, and formation of spatial patterns. Kinetic systems with autocatalysis will be studied using bifurcation theory and other methods of non-linear systems. Kondepudi.

CHM 751. Biochemistry of Nucleic Acids. (1.5-3 h)

Advanced survey of the structure, reactivity, and catalytic properties of RNA and DNA, including modern experimental techniques. Current literature will be presented and critically evaluated.

CHM 752. Protein Chemistry. (1.5-3 h)

Advanced survey of protein biochemistry with an emphasis on structural families, enzyme catalytic mechanisms, expression and purification methods, and biophysical and structural experimental techniques.

CHM 753. Chemical Biology. (3 h)

Survey of the origins and emerging frontiers of chemical biology, with a focus on the impact of chemical methods on our understanding of biology. Topics include protein design, chemical genetics, and methods in genomics and proteomics research.

CHM 755. Biomolecular Mass Spectrometry: Fundamentals and Applications. (1.5-3 h)

Designed for graduate and advanced undergraduates focusing on the principles of mass spectrometry and use in the analysis of small molecules, peptides, proteins, and nucleic acids. Covers sample preparation, data acquisition and interpretation, database searching, and quantification of molecules using a variety of techniques.

CHM 756. Biomolecular NMR. (1.5 h)

One half-semester course designed for graduate and advanced undergraduates focusing on NMR of small oligonucleotides and proteins. Covers sample preparation, data acquisition and processing as well as generating solution structures from NMR data. A student should have command of 1D acquisition and processing as well as experience with 2D acquisition and processing before taking this class. All computational exercises will involve some familiarity with UNIX operating system. P-POI.

CHM 757. Macromolecular Crystallography. (1.5 h)

This is a one-half semester course designed for graduate and advanced undergraduates focusing on structural characterization of macromolecules utilizing x-ray crystallography. The course will cover sample preparation, diffraction theory, data acquisition and processing as well as structure solution and refinement techniques. P-CHM 356A/656 highly recommended.

CHM 761. Chemistry of the Main Group Elements. (3 h)

Principles of bonding, structure, spectroscopy, and reactivity of compounds of the main group elements. Synthesis and applications of organometallic compounds of the main group. Noftle.

CHM 762. Coordination Chemistry. (3 h)

Theory, structure, properties, and selected reaction mechanisms of transition metal complexes. Design and synthesis of ligands and their applications in bioinorganic chemistry. Bierbach, Melson.

CHM 764. Chemical Applications of Group Theory and Symmetry. (3 h)

Symmetry, group theory, bonding, and spectroscopy. Applications to structure, stereoisomers, multicenter bonding and symmetry-controlled reactions. Bierbach, Lachgar, Noftle.

CHM 765. Bioinorganic Chemistry. (3 h)

The inorganic chemistry of life. a) Metals in biocatalysis: elucidation of structure and function of metalloenzymes by various spectroscopic and molecular biology methods; biomimetic ligands; synthetic models of active sites. b) Metals and toxicity. c) Inorganic compounds in therapy and diagnosis. Bierbach.

CHM 771. Quantum Chemistry. (3 h)

The quantum theory and its application to the structure, properties, and interactions of atoms and molecules. Theoretical and computational approaches. Salam, Swofford.

CHM 791. Thesis Research I. (1-9 h)

Staff.

CHM 792. Thesis Research II. (1-9 h)

Staff.

CHM 829. Tutorial in Organic Chemistry. (3 h)

King, Welker, Jones.

CHM 830. Heterocyclic Chemistry. (3 h)

Survey of the major groups of heterocyclic compounds. Modern applications of heterocycles. King.

CHM 831. Principles of Chemical Carcinogenesis. (3 h)

Fundamental chemistry of carcinogenesis. Survey of the chemistry and structure of carcinogenic compounds. Defense and chemotherapeutics.

CHM 832. Theoretical Organic Chemistry. (3 h)

Molecular orbital treatment of structure and reactivity of organic molecules with emphasis on the applications of MO theory in pericyclic and photochemical reactions. Welker.

CHM 833. Advanced Reaction Mechanisms. (3 h)

Detailed analysis of mechanisms with emphasis on characterization of transition state structure.

CHM 838. Advances in Analytical Chemistry - Luminescence Spectroscopy. (3 h)

Instrumentation, methods, and applications of molecular luminescence spectroscopy.

CHM 839. Tutorial in Analytical Chemistry. (2-3 h)

Colyer, Hinze, Jones.

CHM 843. Tutorial in Advanced Kinetics. (3 h)

CHM 844. Tutorial in Thermodynamics/Statistical Mechanics. (3 h)

Kondepudi.

CHM 848. Lasers in Physical Chemistry. (3 h)

Survey of lasers and their use to study physical-chemical processes.

Topics include types of lasers, range of spectral and temporal operation, methods of detection, and application to specific chemical problems.

Swofford.

CHM 849. Tutorial in Chiral Asymmetry in Chemistry and Physics. (3 h)

Chiral asymmetry in nuclear, atomic, and molecular interactions. General group theoretic approach to spontaneous chiral symmetry breaking and the study of specific mechanisms. Kondepudi.

CHM 861. Applications of Electrochemistry. (3 h)

Determination of inorganic and organic reaction mechanisms, electrochemical synthesis, applications to materials science. Noftle.

CHM 862. Special Topics in Coordination Chemistry. (3 h)

Selected applications of transition metal chemistry such as in paramagnetic resonance (NMR, EPR), bioinorganic chemistry, and industrial process. Bierbach, Melson.

CHM 863. Crystallography. (3 h)

Crystal structure determination using powder and single crystal X-ray diffraction. Lachgar.

CHM 864. Modern Chemical Spectroscopy. (3 h)

Applications of vibrational, rotational, electronic, and nuclear spectroscopy to current problems in chemistry. Bierbach, Lachgar, Noftle.

CHM 865. Metallopharmaceuticals. (3 h)

Design and mechanism of metal-containing pharmaceuticals in cancer therapy and diagnosis.

CHM 869. Tutorial in Inorganic Chemistry. (3 h)

Bierbach, Noftle, Lachgar.

CHM 871. Advanced Quantum Chemistry. (3 h)

Advanced quantum mechanical methods for the investigation of electronic structure and radiation-molecule interaction.

CHM 879. Tutorial in Theoretical Chemistry. (3 h)

CHM 888. Dependent Proposal. (3 h)

Course requires a written document detailing the Ph.D. project and an oral exam covering the basic chemical principles, foundation of the plan and experimental design. Pass/Fail. Must be taken before the 6th semester of residence.

CHM 891. Dissertation Research I. (1-9 h)

CHM 892. Dissertation Research II. (1-9 h)

Faculty

Program Director Amanda Jones

Thurmond D. Kitchin Professor of Chemistry and Chair S. Bruce King

John B. White Professor of Chemistry Willie L. Hinze

William L. Poteat Professor of Chemistry Mark E. Welker

Professors Rebecca W. Alexander, Ulrich Bierbach, Christa L. Colyer,

Patricia C. Dos Santos, Bradley T. Jones, Abdessadek Lachgar, Akbar

Salam

Associate Professors Lindsay R. Comstock, Amanda C. Jones, Paul B.

Jones

Assistant Professors Scott M. Geyer, Elham Ghadiri, John C. Lukesh, Troy

A. Stich