Chemistry

Degrees Offered

• Master of Science
• Doctor of Philosophy

Nature of the Program

The Department of Chemistry offers graduate studies leading to the degrees of master of science and doctor of philosophy with research concentration in the areas of analytical, biological, inorganic, organic, and physical chemistry. The master of science and doctor of philosophy degrees require completion of a research project which represents the principal component of the graduate program. The M.S. program is limited in scope and involves advanced coursework and a study of a problem in chemical research culminating in the preparation and oral defense of a M.S. thesis.

The Ph.D. program has a much wider scope than the M.S. program. Ph.D. students are expected to take a broad range of advanced coursework, both within and outside of the major area of interest. The major emphasis of the Ph.D. program is on research. A typical research problem may take several years to complete and involves many advanced techniques and concepts at the frontiers of chemical knowledge. The Ph.D. program culminates in the preparation and defense of the Ph.D. dissertation.

The program for the degree of doctor of philosophy reflects a flexible, research-oriented approach geared to develop the interests, capability, and potential of students. A program of courses is recommended to suit individual needs based on background and ability. These courses are classified as basic graduate courses, which present the essentials of a given discipline on an advanced level, and specialized graduate courses, which take one to the frontiers in a specific area of research. The course offerings are designed to provide guidelines from which students can launch their independent studies in preparation for candidacy examinations. Students are required to enroll in the departmental seminar program and attend special lectures and seminars offered by visiting scientists. Graduate students in the Ph.D. program are required to satisfactorily complete a minimum of three courses (three credits each) at the 500 to 700-level offered by the Department of Chemistry and distributed in at least two areas outside their major area of research. In addition, each major area in chemistry requires students in that area to enroll in basic graduate courses presenting the essentials of that discipline on an advanced level.

FACULTY

CHAIR
• Gregory Dudley - Ph.D. (Massachusetts Institute of Technology)
  Eberly Family Distinguished Professor, Chemical Synthesis, Organic Reaction Methodology, Medicinal Chemistry

PROFESSORS
• Terry Gullion - Ph.D. (William and Mary)
  Physical Chemistry, Solid State NMR, Biological Materials, Polymers
• Lisa Holland - Ph.D. (University of North Carolina-Chapel Hill)
  Micro-separations, High Throughput Drug Screening
• Charles Jaffe - Ph.D. (University of Colorado)
  Theoretical Chemistry, Molecular Dynamics, Chaotic Systems
• Fred L. King - Ph.D. (University of Virginia)
  Analytical Chemistry, Mass Spectrometry, Trace Elements, Gas-phase Chemistry
• Kenneth Showalter - Ph.D. (University of Colorado)
  Bennett Distinguished Professor, Physical Chemistry, Chemical Kinetics, Multistability and Oscillating Systems
• Bjorn C. Soderberg - Ph.D. (Royal Institute of Technology, Sweden)
  Organic Synthesis Using Transition Metals
• Kung K. Wang - Ph.D. (Purdue University)
  Eberly Distinguished Professor of Chemistry, Organic Chemistry, Stereoselective Synthesis, Natural Products

ASSOCIATE PROFESSOR
• Fabien Goulay - Ph.D. (University of Rennes, France)
  Physical Chemistry, Laser Spectroscopy
• Justin Legleiter - Ph.D. (Carnegie Mellon University)
  Biophysical Chemistry, Scanning Probe Microscopy
• Michelle Richards-Babb - Ph.D. (Lehigh University)
  Chemical Education
• Stephen Valentine - Ph.D. (Indiana University)
  Mass Spectrometric Analysis of Biomolecules

ASSISTANT PROFESSOR
• Jessica Hoover - Ph.D. (University of Washington)
  Organometallic Chemistry, Catalysis
• Peng Li - Ph.D. (Texas Tech University)
  Bioanalytical Chemistry
• Blake Mertz - Ph.D. (Iowa State University)
  Computational Biophysics and Chemistry
• Carsten Milsmann - Ph.D. (Max-Planck-Institute for Bioinorganic Chemistry)
  Inorganic and Organometallic Chemistry
• Brian Popp - Ph.D. (University of Wisconsin-Madison)
  Organic and Organometallic Chemistry, Catalysis

Admission
Applicants for graduate studies in chemistry must have a bachelor's degree as a minimum requirement. Applicants must have a major or concentration in chemistry and an appropriate background in physics and mathematics. All entering graduate students in chemistry are required to take departmental guidance examinations in the major areas of chemistry. These examinations, at the undergraduate level, are administered before registration and serve to guide the faculty in recommending a course program for the beginning graduate student. Deficiencies revealed by the departmental guidance examinations need to be corrected in a manner prescribed by the faculty.

Master of Science
A research project is chosen in the area of the student's interest and in consultation with the faculty. The thesis defense shows the ability of the student to defend scientific conclusions based on their research project.

MAJOR REQUIREMENTS
Minimum GPA of 3.0 is required.

<table>
<thead>
<tr>
<th>Coursework</th>
<th>Hours</th>
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<tbody>
<tr>
<td>Chemistry Coursework (400, 500, 600, 700-level)</td>
<td>22</td>
</tr>
<tr>
<td>Research</td>
<td>6</td>
</tr>
<tr>
<td>CHEM 797 Research (Repeated)</td>
<td></td>
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<tr>
<td>CHEM 796 Graduate Seminar</td>
<td>1</td>
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<tr>
<td>CHEM 789 Research Seminar</td>
<td>1</td>
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<tr>
<td>Thesis</td>
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<tr>
<td>Thesis Defense</td>
<td></td>
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<tr>
<td>Total Hours</td>
<td>30</td>
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Thesis/Credits
Graduate students in the M.S. program in chemistry are required to submit a research thesis. They may apply up to 6 hours of research credit toward the 30-hour requirement. The remaining 24 hours of credit must be earned in the basic graduate courses which reflect a diversified exposure to chemistry; no more than 10 hours may be elected outside the department, and coursework taken at the 500 to 700-level must include at least three 3-credit-hour courses distributed in at least two areas outside the student's major area of research. Students are required to enroll in the departmental seminar program and are required to attend special lectures and seminars offered by visiting scientists. A final oral examination is administered after completion and submission of the thesis.

Doctor of Philosophy
Students are required to enroll in the departmental seminar program and attend special lectures and seminars offered by visiting scientists. In addition, each major area in chemistry requires students in that area to enroll in basic graduate courses presenting the essentials of that discipline on an advanced level.

MAJOR REQUIREMENTS
Minimum GPA of 3.0 is required.

<table>
<thead>
<tr>
<th>Coursework</th>
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<tbody>
<tr>
<td>Chemistry Coursework (500, 600, 700-level)</td>
<td>18</td>
</tr>
<tr>
<td>Graduate Research</td>
<td>24</td>
</tr>
<tr>
<td>CHEM 797 Research (Repeated)</td>
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### Research

Research, which is the major theme of graduate studies, may be initiated as early as the student and faculty feel appropriate for the individual. Normally, a student will begin laboratory work no later than the beginning of the second semester. Upon successful completion of an original piece of research, the candidate will present results in a Ph.D. dissertation and, at the appropriate time, defend the work in a final oral examination.

### Candidacy

Candidacy examinations contain written and oral portions. The written portion is a research progress report that will contain a comprehensive review of the pertinent literature and applicable scientific concepts, a discussion of current results, a description of studies needed to finish the project, a discussion of expected results and alternative approaches, and a timeline for completing the work. After notification of successful completion of the written portion, the student will present and defend an oral progress report. This oral report must demonstrate fundamental chemical knowledge and independence on the part of the student. Both the written and oral portions of the candidacy examination will be evaluated by the student’s research committee and any other interested faculty members.

### Major Learning Outcomes

**CHEMISTRY**

The graduate programs in the C. Eugene Bennett Department of Chemistry provide rigorous training in chemistry. The central mission of the Graduate Program is to train the next generation of Chemists for productive careers in the global economy.

Students earning a M.S. or Ph.D. in Chemistry will be able to:

- Explain chemical principles as they pertain to their specific field of research.
- Demonstrate the ability to understand and critically evaluate the existing literature published within their field.
- Independently design and execute new chemical experiments that can address important scientific questions.
- Understand and apply good laboratory practices (chemical hygiene, personal protective wear, etc.) and the proper handling of chemical waste streams.
- Generate quality data using a variety of experimental and/or computational techniques.
- Interpret the meaning and implication of their data.
- Effectively communicate their research in oral and written formats, including the ability to author manuscripts suitable for publication in peer reviewed scientific journals.
- Understand the ethical impact of personal and professional behavior.

### COURSES

**CHEM 511. Advanced Instrumental Analysis. 3 Hours.**
PR: CHEM 310 with a minimum grade of C-. Lectures and demonstrations. Classical and cutting-edge instrumental methods applied to chemical analyses: electrochemistry, spectroscopy, mass spectrometry, and chromatography; presented at the advanced level. (3 hr. lec.).

**CHEM 512. Environmental Chemistry. 3 Hours.**

**CHEM 514. Mass Spectrometry Principles and Practices. 3 Hours.**
PR: CHEM 310. Fundamental principles underlying modern mass spectrometry. Gas phase chemistry related to the formation and fragmentation of ions. The design of instrumental systems for mass spectrometry. Application of mass spectrometric techniques to multidisciplinary problems of current interest. (3 hr. lec.).

**CHEM 516. Bioanalytical Chemistry. 3 Hours.**
PR: (CHEM 310 and AGBI 410) or equivalent. Analytical principles and instrumental methods as they are applied to biochemical questions. Students are taught to evaluate and formulate methods and approaches for biochemical analyses.
CHEM 521. Organometallic Chemistry. 3 Hours.
PR: Graduate standing in chemistry or consent. Syntheses, structure, and reactivity of organometallic compounds. Applications of organometallic compounds to catalysis and organic synthesis. (3 hr. lec.).

CHEM 522. Topics in Inorganic Chemistry. 3 Hours.
Structure and bonding of inorganic molecules and materials. Covers the chemistry of main group elements and transition metals. Application of fundamental principles in inorganic chemistry to current research problems.

CHEM 531. Advanced Organic Chemistry 1. 3 Hours.
PR: CHEM 234. Structural concepts, bonding, tautomerism, static and dynamic stereochemistry, mechanistic classifications of reagents, and reactions including some applications. (3 hr. lec.).

CHEM 532. Advanced Organic Chemistry 2. 3 Hours.
PR: CHEM 531. Continuation of CHEM 531 with emphasis upon synthetic methods and reaction mechanisms. (3 hr. lec.).

CHEM 533. Advanced Structure Determination Using Spectroscopic Methods. 3 Hours.
PR: Graduate standing or consent. In depth exposure to the techniques for identifying the functionalities and elucidating the bond connectivity of unknown organic molecules using UV, IR, and NMR spectroscopy and mass spectrometry techniques.

CHEM 540. Bonding and Molecular Structure. 3 Hours.
PR: CHEM 348. Introduction to the quantum theory of chemical bonding. Atomic structure, theoretical spectroscopy, predictions of molecular structures and bond properties. (3 hr. lec.).

CHEM 541. Chemical Thermodynamics. 3 Hours.
PR: CHEM 348. Principles of classical and statistical thermodynamics and their application to chemical problems. (3 hr. lec.).

CHEM 542. Computational Chemistry. 3 Hours.
PR: CHEM 348 or consent. Introduction to the use of quantum mechanical-based computational techniques to study molecular structure, bonding, and reactivity, and their relationship to experimental techniques.

CHEM 545. Foundations of Quantum Chemistry. 3 Hours.
Application of the principles of quantum mechanics to chemical systems and spectroscopy.

CHEM 547. Chemical Crystallography. 3 Hours.
PR or Conc: (CHEM 346 and CHEM 348) or CHEM 341 or consent. Applications of X-ray diffraction of crystals to the study or crystal and molecular structure. Includes diffraction theory, space group symmetry, and crystallographic methods of analysis. (3 hr. lec.).

CHEM 548. Biophysical Chemistry. 3 Hours.
Biophysical Chemistry lies at the interface between physics, chemistry and biology, applying theories and methods of the physical sciences toward understanding biological systems. This course focuses on the physical chemistry of biological macromolecules. Topics to be covered include protein structure formation and stability, forces/interactions in biological molecular systems, bio-macromolecule folding dynamics, phase transitions in proteins, and membrane physics.

CHEM 549. Proximal Probe Techniques. 3 Hours.
Proximal probe techniques rely on the use of nanoscale probes, positioned and scanned in the immediate vicinity of surfaces. Their development is often viewed as a first step towards nanotechnology, since they demonstrate the feasibility of building purposeful structures one atom or one (macro) molecule at a time. This course provides thorough physical background of scanning probe microscopy techniques.

CHEM 552. Biochemical Toxicology. 3 Hours.
Introduction to the principles of toxicology, with a focus on the processes that occur at the cellular and molecular levels when chemicals interact with living organisms.

CHEM 591A-U. Advanced Topics. 1-6 Hours.
CHEM 591U. Advanced Topics. 1-6Hr. PR: Consent. Investigation of advanced topics not covered in regularly scheduled courses.

CHEM 593A-Z. Special Topics. 1-6 Hours.
A study of contemporary topics selected from recent developments in the field.

CHEM 697. Research. 1-15 Hours.
PR: Consent. Research activities leading to thesis, problem report, research paper or equivalent scholarly project, or a dissertation. (Grading may be S/U.).

CHEM 713. Electrochemistry and Instrumentation. 3 Hours.
PR: CHEM 310. Electronic instrumentation applied to study of mass transfer kinetics of electrode reactions, voltammetry, and high-frequency methods. (3 hr. lec.).

CHEM 714. Analytical Atomic Spectrometry. 3 Hours.
PR: CHEM 450. Theory of atomic spectroscopy relevant to elemental analysis. Considerations in the design and use of modern optical spectrometry systems. (3 hr. lec.).

CHEM 715. Chemical Separations. 3 Hours.
PR: CHEM 215 and CHEM 233, and physical chemistry. Fundamentals of transport and flow processes underlying all separation techniques. Empirical coverage of chromatographic and electrophoretic methods for analytical separations. (3 hr. lec.).
CHEM 723. Physical Methods in Inorganic Chemistry. 3 Hours.
PR: CHEM 422. Symmetry, vibrational spectroscopy, theory and applications of NMR and EPR methods, magnetism, optical activity, dynamic processes and fluxional behavior. (3 hr. lec.).

CHEM 724. Coordination Chemistry. 3 Hours.
PR: CHEM 422. Symmetry, hybridization, ligand field theory, molecular orbital theory, metal-ligand bonding in coordination complexes and organometallics. (3 hr. lec.).

CHEM 725. Inorganic Reactions and Mechanisms. 3 Hours.
PR: CHEM 422. Inorganic reactions (ligand substitution aquation, organometallic reactions, electron transfer;) kinetics and mechanistic studies. (3 hr. lec.).

CHEM 727. Bioinorganic Chemistry. 3 Hours.
PR:CHEM 422 or consent. Metal ions in biological systems; proteins, nucleic acids, and cofactors as ligands; metal uptake, storage, and regulation; structural and catalytic roles; substance activation, electron transfer, and group transfer reactions; metals in medicine.

CHEM 733. Physical Organic Chemistry. 3 Hours.
PR: CHEM 531. Theoretical considerations of organic molecules, kinetics, and other methods used in the study of organic structure and reaction mechanisms; linear free energy relationship and other related topics. (3 hr. lec.).

CHEM 743. Chemical Kinetics. 3 Hours.
PR: CHEM 348. Theories and applications of kinetics in gaseous state and in solution. (3 hr. lec.).

CHEM 744. Statistical Mechanics. 3 Hours.
PR: CHEM 746. Theory and application of statistical mechanics to chemical systems. (3 hr. lec.).

CHEM 745. Theoretical Chemistry 1. 3 Hours.
PR: Differential equations. Theoretical background for quantum mechanics. (3 hr. lec.).

CHEM 746. Theoretical Chemistry 2. 3 Hours.
PR: CHEM 745. Theories and applications of quantum mechanics in chemistry. (3 hr. lec.).

CHEM 747. Molecular Spectroscopy and Structure. 3 Hours.
PR: CHEM 450 or graduate standing in chemistry, or consent. Advanced applications of spectral methods to the study of molecular structure. (3 hr. lec.).

CHEM 750. Introduction to Proteomics. 3 Hours.
Introduction to protein separations and sequencing by modern mass spectrometry, and the application of these methods to the study of biological systems in health and environmental sciences.

CHEM 789. Research Seminar. 1 Hour.
PR: Graduate student in chemistry. Research seminars by visiting lecturers.

CHEM 790. Teaching Practicum. 1-3 Hours.
PR: Consent. Supervised practice in college teaching of chemistry. Note: This course is intended to insure that graduate assistants are adequately prepared and supervised when they are given college teaching responsibility. It will also present a mechanism for students not on assistantships to gain teaching experience. (Grading will be P/F.).

CHEM 791A-Z. Advanced Topics. 1-6 Hours.
PR: Consent. Investigation of advanced topics not covered in regularly scheduled courses.

CHEM 792A-Z. Directed Study. 1-6 Hours.
Directed study, reading, and/or research.

CHEM 793A-Z. Special Topics. 1-6 Hours.
A study of contemporary topics selected from recent developments in the field.

CHEM 794A-Z. Special Seminar. 1-6 Hours.
Seminars arranged for advanced graduate students.

CHEM 795. Independent Study. 1-9 Hours.
Faculty supervised study of topics not available through regular course offerings.

CHEM 796A-C. Graduate Seminar. 1 Hour.
PR: Consent. It is anticipated that each graduate student will present at least one seminar to the assembled faculty and graduate student body of his/her program.

CHEM 797. Research. 1-15 Hours.
PR: Consent. Research activities leading to thesis, program report, research paper or equivalent scholarly project, or a dissertation. (Grading may be S/U.).

CHEM 798. Thesis or Dissertation. 1-6 Hours.
PR: Consent. This is an optional course for programs that wish to provide formal supervision during the writing of student reports (698), or dissertations (798). Grading is normal.
CHEM 799. Graduate Colloquium. 1-6 Hours.
PR: Consent. For graduate students not seeking coursework credit but who wish to meet residency requirements, use of the University's facilities, and participate in its academic and cultural programs. Note: Graduate students who are not actively involved in coursework or research are entitled, through enrollment in their department's 699/799 Graduate Colloquium to consult with graduate faculty, participate in both formal and informal academic activities sponsored by their program, and retain all of the rights and privileges of duly enrolled students. Grading is P/F; colloquium credit may not be counted against credit requirements for masters programs. Registration for one credit of 699/799 graduate colloquium satisfies the University requirement of registration in the semester in which graduation occurs.