

Chemistry (Ph.D., M.S)

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Prospective students should use this checklist to obtain specific admissions requirements on how to apply to Graduate School.

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Degree Offered:	Ph.D., M.S.
Director:	<i>David E. Graves</i>
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Faculty

Venkatram R. Atigadda, Research Assistant Professor (Chemistry); Organic Chemistry, Synthesis, drug design and synthesis, anticonvulsant drug development, antidiabetic and cardiac drug development, drugs for treating or preventing cancer, drugs for influenza.

Christie G. Brouillette, Research Professor (Chemistry); Biophysical Chemistry, protein structural cooperativity and energetics through the application of biophysical techniques to study protein stability and protein-ligand interactions, with particular emphasis on pharmaceutical development.

Wayne J. Brouillette, Professor (Chemistry); Design and synthesis of small organic molecules as new drugs. Active projects include neuraminidase inhibitors as drugs for influenza; NAD synthetase inhibitors as biological warfare defense agents and broad spectrum antibacterial agents; sodium channel ligands as neuroprotective (anti-stroke), analgesic, and anticancer agents; and retinoids as chemopreventive and chemotherapeutic agents. Combinatorial chemistry, structure-based drug design, and computer-assisted methods such as in silico screening (FlexX) and 3D-QSAR (CoMFA) are utilized.

David E. Graves, Professor and Chair (Chemistry); Biophysical Chemistry, nucleic acid structure and function, interactions of ligand-DNA interactions, development of novel topoisomerase I and II inhibitors for cancer chemotherapy.

Gary M. Gray, Professor (Chemistry); Inorganic Chemistry, Transition metal P-donor complexes, chemistry of metallacrown ethers, transition metal complexes that combine the catalytic abilities of transition metal complexes of phosphorus-donor ligands with the cation and small molecule binding abilities of crown ethers, synthesis of metal containing polymers for use in laser fusion, transition metal complexes can exhibit third-order optical nonlinearities.

Tracy P. Hamilton, Associate Professor (Chemistry); Physical Chemistry, *Ab Initio* theoretical chemistry development and applications, reactions of nitric oxide (NO) with superoxide (O₂⁻). Predictions of the vibrational spectroscopy of peroxyxynitrite and its salts, the UV- visible electronic spectrum, the NMR shifts, the energetics, and the reactions of peroxyxynitrite with other molecules such as carbon dioxide.

Eugenia Kharlampieva, Assistant Professor (Chemistry)

Aaron L. Lucius, Assistant Professor (Chemistry); Biophysical Chemistry, Kinetic and thermodynamic methods to examine catalyzed protein unfolding, DNA helicase and DNA gyrase mechanisms.

Craig P. McClure, Assistant Professor (Chemistry); Chemical Education, development of novel chemistry instruction pedagogy, enhancement of retention in introductory chemistry for nonscience majors.

Donald D. Muccio, Professor (Chemistry); Biophysical Chemistry, the use and interpretation of spectroscopy, including NMR and circular dichroism CD to probe structures, folding, and ligand binding of conformationally constrained retinoids, peptides that damage the cornea in the alkaline-injured eye, and NAD synthetase - a new target for antibacterial agents.

Jacqueline A. Nikles, Associate Professor (Chemistry); Chemical Education, development of novel methods for enhancing organic chemistry instruction and student retention.

James C. Patterson, Assistant Professor (Chemistry); Computational methods to study the reaction mechanisms of metalloenzymes and the dynamic of membrane-associated proteins.

Sadanandan E. Velu, Assistant Professor (Chemistry); Organic Synthesis, total synthesis of natural compounds with biological activities, development of novel topoisomerase I and II inhibitors, antibacterial drug development.

Sergey Vyazovkin, Associate Professor (Chemistry); Analytical Chemistry. Thermophysical properties and reactions of polymeric, energetic, and pharmaceutical materials using a variety of analytical techniques including Infrared (IR) spectroscopy, Mass Spectrometry (MS), Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC), Thermomechanical Analysis (TMA), Dynamic Mechanical Analysis (DMA), Polarized Light Microscopy (PLM). Kinetic analysis of thermal data plays the key role in our work. We develop and apply our original kinetic methodology known as "Model-free Kinetics".

Pengfei Wang, Assistant Professor (Chemistry); Organic Chemistry, Discovery and development of new methods and their application toward prodrug design and synthesis, carbohydrate chemistry, and synthesis of biologically important natural products. The main focus centers on the development of new reactions and methodologies which would lead to general, flexible and dependable approaches to various synthetic and medicinal targets.

Program Information

General Requirements

The graduate curricula in the Department of Chemistry are designed to ensure superior disciplinary quality and research competency in target research areas that UAB can uniquely offer. This department has an outstanding research active faculty that provides a very favorable faculty/student ratio to encourage close contacts between students and their faculty research advisors and provides opportunities for mentors to give personalized attention to the academic and research progress of each of their students.

All graduate students are required to pursue a graduate curriculum that provides the general knowledge-based foundation for the student's program through a series of six core curriculum courses (18 semester hours). All students are required to enroll in two Foundations Courses [CH 700, Foundations I (Analytical and Physical); CH 701, Foundations II (Organic and Inorganic)] and four additional courses that they may select to complete their course requirements. Graduate students also enroll in courses offered in the Basic Health Sciences and the Joint Material Sciences Programs to broaden their backgrounds in selective areas and greatly strengthen their ability to carry out interdisciplinary research. Students involved in interdisciplinary programs (pharmaceutical design, materials science, molecular biophysics, forensic science, etc.) may, with the approval of their Advisory Committee, make appropriate substitutions for some of the courses, i.e. Polymer/Materials Chemistry, Biochemistry, etc. A grade of B must be earned in each of these courses for Admission to Candidacy in the Ph.D. program. Courses may be repeated once to raise the grade.

All graduate students are to demonstrate communication skills competencies. Adequate performance is required on the literature seminar, written responses to essay exams, dissertation defense, teaching, written publications, presentations at professional meetings, and/or enrollment in the Graduate School course series GRD 701 (Presentation and Discussion Skills), GRD 702 (Writing Up Research), and GRD 717 (Principles of scientific integrity). All incoming international graduate students will be required to take GRD 700 (Culture and speaking in the US as well as GRD 714 (Individualized Pronunciation and Accent Training). All graduate students are required to present a departmental literature seminar after their first year.

Students must select a research advisor after their first year and have a research committee in place by the end of their third semester. This selection occurs after the student has interviewed each graduate faculty member in the Department of Chemistry. The student and the major professor will recommend to the director of the graduate program in chemistry the composition of the graduate study committee.

Core Courses: CH 629/729, CH 631/731, CH 632/732, CH 633/733, CH 639/739, CH 642/742, CH 649/749, CH 659/759, CH 664/764, CH 669/769, CH 671/771, CH 689/789

Substitutions are permitted with the approval of the student's research advisory committee and director of the graduate program.

Master's students choose from the 600 courses, Ph.D. students from the 700 courses.

M.S. Program

Plan I

Plan I is a research program that requires a minimum of 24 semester hours (including 18 semester hours of core courses) of formal academic coursework approved by the student's graduate study committee. The progress of the student's research program is monitored by the graduate study committee. The student, having been admitted to candidacy and having completed an approved plan of research, will complete and defend a thesis.

Plan II

Plan II is a nonthesis program that requires a minimum of 30 semester hours (including 18 semester hours of core courses) of appropriate graduate work that has been approved by the student's graduate study committee.

Ph.D. Program

For Ph.D. students, there are no specific course requirements beyond the core courses. The academic program is determined through the action of the student's graduate study committee. A written qualifying examination must be passed in the student's area of specialization. If failure occurs, only one repeat exam is allowed. A research proposal must be defended within 12 months of completion of the written qualifying examination. If failure occurs, one repeat defense is allowed. The student, having been admitted to candidacy and having completed an approved plan of research, will submit a dissertation to the Graduate School. This dissertation must be defended at an open meeting. **Additional Information**

NIBIB Supported T-32 Predoctoral Training Grant

National Institute of Biomedical Imaging and Bioengineering (NIBIB) has awarded an interdisciplinary predoctoral training grant to UAB that is entitled "Nanotechnology in Biosensors and Bioengineering". It is a five year program that started on September 1, 2007. Benefits to participating graduate students include: graduate stipends of \$25,000 per year, full tuition and health insurance, and a travel award of \$1,000 per year. The purpose of this grant is to implement a training program at the interfaces of physics, chemistry, materials science and engineering, and biomedical engineering that will reduce the time from discovery of a new tool in nanotechnology to its application in medical devices, tissue engineering, and biosensors for earliest detection of molecular signatures of disease.

For more information regarding this training program, visit <http://www.uab.edu/cnmb/graduate/index.html>.

Deadline for Entry Term(s):	Each semester
Deadline for All Application Materials to be in the Graduate School Office:	Six weeks before term begins
Number of Evaluation Forms Required:	Three
Entrance Tests	GRE (TOEFL and TWE also required for international applicants whose native language is not English.)

Comments	None
Graduate Catalog Description	http://main.uab.edu/show.asp?durki=24862

For detailed information, contact Dr. David E. Graves, Department of Chemistry Graduate Program Director, CHEM 201C, 1530 3rd Avenue South, Birmingham, AL 35294-1240.
Telephone 205-975-8094

E-mail dgraves@uab.edu

Web www.chem.uab.edu

Course Descriptions

Unless otherwise noted, all courses are for 3 semester hours of credit. Course numbers preceded with an asterisk indicate courses that can be repeated for credit, with stated stipulations.

Chemistry (CH)

525. Physical Chemistry I for Graduate Study. Thermodynamics and chemical equilibria; and chemical kinetics. Prerequisites: MA 126, PH 202, CH 117. Fall.

526. Physical Chemistry II for Graduate Study. Quantum mechanics, chemical bonding, and molecular spectroscopy. Prerequisite: CH 525. Spring.

535. Organic Chemistry I for Graduate Study. Structure of organic compounds based on bonding, stereochemical, and physical properties. Fall, spring, summer.

537. Organic Chemistry II for Graduate Study. Practical and theoretical considerations of organic reactions; Introduction to spectroscopy. Prerequisite: CH 535. Fall, Spring, Summer.

540. Inorganic Chemistry I for Graduate Study. Chemical reactivity and descriptive chemistry in terms of structural and electronic parameters. Fall.

541. Transition Metal Chemistry. Atomic structure, chemical bonding characterization and reactivity of transition metal complexes. Prerequisite: CH 345, CH 326. Spring.

550. Analytical Chemistry I for Graduate Study. Analytical measurements, spectrophotometric and gravimetric analyses, chromatography, and chemical equilibrium. Spring.

555. Analytical Chemistry II for Graduate Study. General operating principles and quantitative applications of commonly used analytical instruments. Prerequisite: CH 550. Spring.

561. Biochemistry I: Introduction to biological macromolecules and chemistry and physical properties of component building blocks. Prerequisites: 237 and 355. Successful completion of CHEM 561 is a prerequisite for CHEM 562. Fall.

562. Biochemistry II. Continuation of biochemistry including molecular genetics (replication, transcription, and translation), metabolic pathways, control of gene expression. Prerequisite: 561. Spring.

563. Biochemistry Laboratory. Introduction to modern analytical techniques used for the isolation and characterization of biological macromolecules. Prerequisites: CH 355 and CH 461 and permission of instructor.

564. Physical Biochemistry Laboratory. Physical/analytical approaches toward determination of macromolecular structures, ligand binding, and enzymology. Prerequisites: CH 325, CH 355, and CH 461 or permission of instructor.

580. Polymer Chemistry I. (also MSE 530). Structure and properties of crystalline and amorphous polymers; polymer processing; correlation of polymer structure with processability and performance. Synthesis and characterization of polymers; polymerization reactions, kinetics, and mechanisms; polymer solution properties. Prerequisite: CH 237, 325, or MSE 254. Spring.

581. Polymer Chemistry II. Synthesis and characterization of polymers: polymerization reaction kinetics and mechanisms; polymer solution properties. Prerequisite: CH 580 and concurrent enrollment in CH 581L.

600. Foundations of Physical and Analytical Chemistry. Molecular thermodynamics and molecular reaction dynamics, chemical equilibrium and solubility in aqueous/organic solutions, and ligand binding to macromolecules in aqueous solution. Fall.

601. Foundations of Organic and Inorganic Chemistry. Organic – Bonding and structure, concerted pericyclic reactions, stereochemistry, effects of conformation, sterics and electronics on reactivity; and the study of reaction mechanisms with emphasis on nucleophilic substitution. Inorganic – Bonding and structure including basic molecular orbital theory, the solid state, Lewis acid-base chemistry, coordination chemistry, reaction mechanisms for transition metal complexes and characterization of transition metal complexes.

602. Principles of Chemical Instruction. Responsibilities of laboratory instructors, safety regulations, grading, teaching styles and formats, and instructional objectives. Prerequisite: Permission of instructor. Fall. 1 hour.

610. Laboratory Experiences in Chemistry I. Application of simple experiments to high school science programs.

611. Laboratory Experiences in Chemistry II. Continuation of CH 602.

612. Polymer Chemistry for Teachers. Lecture and laboratory experiences focusing on natural and synthetic polymers. Morning lectures by polymer chemists with afternoon labs where polymers are synthesized and studied. Emphasis is on practical application and new developments in polymer chemistry. Experiments are suitable for high school science programs.

613. Introductory Organic Chemistry for Teachers. A laboratory, lecture, demonstration course on the nature of carbon compounds including hydrocarbons, functional groups and their reactions. Emphasis given to laboratory experiments and demonstrations suitable for high school students.

614. Introductory Biochemistry for Teachers. Lecture series covering carbohydrates, lipids, and proteins. Emphasis given to practical applications and relationship between chemistry and biology. Aspects of nutrition are discussed.

615. Introductory Biochemistry for Teachers II. Lecture series covering vitamins, minerals, enzymes, biochemical energy and metabolism. Strong connections between chemistry and biology. Practical applications are emphasized.

616. Chemical Demonstrations. A laboratory-based course exploring the teaching potential of selected chemical reactions. Teachers perform at least 50 demonstrations in the laboratory and share ways they can use these in their own classes. Emphasis on facilitating learning of chemistry.

617. Chemical Demonstrations II. At least 50 demonstrations will be performed. Focus is on safe, practical and effective experiments suitable for high school students.

619. Special Topics in Chemical Education. Topics determined by interest of students and faculty.

625. Molecular Structure and Spectroscopy. Classical and quantum mechanical descriptions of molecular structure and bonding. Basic principles and techniques of molecular spectroscopic methods. Exercises and experiments with computational software and spectroscopic instrumentation will be conducted.

629. Special Topics in Physical Chemistry. Topics determined by interest of s students and faculty. Typical are computational chemistry, molecular spectroscopy, nuclear magnetic resonance. Prerequisite: CH 600 or permission of Instructor. 1 – 3 hours.

630. Physical Organic Chemistry. Localized and delocalized chemical bonds, stereochemistry, acidity and basicity, determining organic mechanisms and structure. Fall.

631. Organic Reactions and Their Mechanisms. Nucleophilic and electrophilic substitution, free radical substitutions, additions to carbon-carbon and carbon-hetero multiple bonds, elimination reactions. Prerequisite: CH 730. Spring.

632. Organic Reactions and Synthesis. Strategy of synthesis, carbon skeletal assembly, selective functional group interconversion, blocking groups, stereochemical control. Prerequisite: CH 731. Spring.

633. Reactive Intermediates and Conservation of Bonding. Behavior of organic molecules in static and reactive situations. Prerequisite: CH 731 or permission of instructor. Spring.

639. Special Topics in Organic Chemistry. Topics determined by interest of students and faculty. Prerequisite: CH 327. 1-3 hours.

640. Bonding and Structure in Inorganic Compounds. Advanced treatment of bonding in main group and transition metal compounds, and a study of its relationship to the properties of compounds. Prerequisite: CH 540 or permission of instructor. Spring.

642. Organometallic Chemistry and Catalysis. Study of transition metal organometallic compounds and their applications as homogeneous catalysts for organic and polymer syntheses. Prerequisite: CH 640 or 740 or permission of instructor. Summer (alternate years).

649. Special Topics in Inorganic Chemistry. Topics determined by interest of students and faculty. Prerequisite: Permission of instructor. 1-3 hours.

650. Chemometrics. Introduction to basic data analysis techniques that include testing hypotheses, establishing tendencies and correlations, experimental design, etc. The course is designed to provide a support to a research chemist in effectively solving everyday problems associated with production and interpretation of experimental data. Prerequisite: Permission of instructor.

659. Thermal processes and methods. Introduction to thermally initiated physical and chemical processes in the condensed phase systems such as liquids, crystalline solids, and glasses (amorphous solids). The course covers the use of calorimetry, thermogravimetry, and thermomechanical methods for exploring thermodynamics and kinetics of crystallization, glass transition, solid-solid and helix-coil transitions, decomposition, polymerization, etc. Prerequisite: permission of instructor.

664. Biophysical Chemistry. Common physical methods for understanding the structure and stability of macromolecules that include several spectroscopic, thermodynamic and computational methods. Underlying physical principle described, instrumentation discussed, and examples cited from the literature. Prerequisite: CH 325 or 461. Spring.

669. Special Topics in Biochemistry. Detailed consideration of areas of special interest. Prerequisite: CH 462.

670. Chemical Literature. Use of on-line literature and development of searching techniques.

671. Medicinal Chemistry & Drug Discovery. Description. Emphasis on design strategies for small organic drugs using common macromolecular drug targets. Examples of successful design for clinically used drug classes will be presented. Prerequisites include undergraduate organic chemistry (CH235 and CH237) and undergraduate biochemistry (CH461) or equivalent.

689. Special Topics in Polymer Chemistry. Detailed consideration of areas of special interests in polymer chemistry. Prerequisite: CH 580, 581.

691. Seminar. Seminars on current topics in chemical research. Pass/Fail. 1 hour.

692. Seminar Presentation. Seminar given by graduate students on current topics in chemical research. 2 hours.

698. Graduate Research. Prerequisite: Permission of graduate faculty member. Pass/Fail. 1-8 hours.

699. M.S. Thesis Research. Prerequisites: Admission to candidacy and permission of graduate faculty member. 1-8 hours.

700. Foundations of Physical and Analytical Chemistry. Molecular thermodynamics and molecular reaction dynamics, chemical equilibrium and solubility in aqueous/organic solutions, and ligand binding to macromolecules in aqueous solution. Fall.

701. Foundations of Organic and Inorganic Chemistry. Organic – Bonding and structure, concerted pericyclic reactions, stereochemistry, effects of conformation, sterics and electronics on reactivity; and the study of reaction mechanisms with emphasis on nucleophilic substitution. Inorganic – Bonding and structure including basic molecular orbital theory, the solid state, Lewis acid-base chemistry, coordination chemistry, reaction mechanisms for transition metal complexes and characterization of transition metal complexes.

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faculty. Prerequisite: Permission of instructor. 1-3 hours.

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792. Seminar Presentation. Seminar given by graduate students on current topics in chemical research. 2 hours.

798. Nondissertation Research. Prerequisite: Permission of graduate faculty member. Pass/Fail. 1-8 hours.

799. Dissertation Research. Prerequisite: Admission to candidacy and permission of graduate faculty member. 1-8 hours.

Last modified 03/16/11