Chemistry

Degrees Offered
• Master of Science (Chemistry; thesis and non-thesis options)
• Doctor of Philosophy (Applied Chemistry)

Program Description
The Department of Chemistry offers MS (thesis and non-thesis options) in Chemistry and PhD degrees in Applied Chemistry. In addition, interdisciplinary MS and PhD degrees are also offered in Geochemistry, Hydrological Sciences and Engineering, Materials Science, Nuclear Engineering, and Quantitative Biosciences and Engineering.

Prerequisites
A candidate for an advanced degree in the Chemistry program should have completed an undergraduate program in Chemistry which is essentially equivalent to that offered by the Department of Chemistry at the Colorado School of Mines. Undergraduate deficiencies will be determined by faculty in the Department of Chemistry through interviews and/or placement examinations at the beginning of the student's first semester of graduate work.

WICHE
All graduate degree programs in the Department of Chemistry have been admitted to the Western Regional Graduate Program (WICHE). This program allows residents of Alaska, Arizona, California, Hawaii, Idaho, Montana, Nevada, New Mexico, North Dakota, Oregon, South Dakota, Utah, Washington, and Wyoming to register at Colorado resident tuition rates.

Required Curriculum
Chemistry
A student in the chemistry program, in consultation with the advisor and thesis committee, selects the program of study. Initially, before a thesis advisor and thesis committee have been chosen, the student is advised by a temporary advisor and by the Graduate Affairs Committee in the Department of Chemistry.

MS Degree (chemistry, thesis option): The program of study includes coursework, research, and the preparation and oral defense of an MS thesis based on the student’s research. The required courses are:

<table>
<thead>
<tr>
<th>Course Code</th>
<th>Course Title</th>
<th>Credits</th>
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</thead>
<tbody>
<tr>
<td>CHGN502</td>
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<td>3.0</td>
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<tr>
<td>CHGN503</td>
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<td>3.0</td>
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<tr>
<td>CHGN560</td>
<td>GRADUATE SEMINAR, M.S. (M.S.-level seminar)</td>
<td>1.0</td>
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Students should enroll in CHGN560 in the first semester of their degree program. A minimum of 36 semester hours, including at least 24 semester hours of course work, are required. At least 15 of the required 24 semester hours of course work must be taken in the Department of Chemistry at Mines. The student’s thesis committee makes decisions on transfer credit. Up to 9 semester hours of graduate courses may be transferred from other institutions, provided that those courses have not been used as credit toward a Bachelor’s degree.

Research-Intensive MS Degree: Mines undergraduates who enter the graduate program through the combined BS/MS program may use this option (thesis-based MS) to acquire a research-intensive MS degree by minimizing the time spent on coursework. This option requires a minimum of 12 hours of coursework up to six hours of which may be double counted from the student’s undergraduate studies at Mines (see below).

MS Degree (chemistry, non-thesis option): The non-thesis MS degree requires 30 semester hours of course credit:

<table>
<thead>
<tr>
<th>Course work</th>
<th>Independent study</th>
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<tr>
<td>24.0</td>
<td>6.0</td>
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</table>

Total Semester Hrs: 30.0

The program of study includes coursework, independent study on a topic determined by the student and the student’s faculty advisor, and the preparation of an oral presentation of a report based on the student’s independent study topic. The required courses are:

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</tr>
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Total Semester Hrs: 13.0

Students should enroll in CHGN560 in the first semester of their degree program. At least 21 of the required 30 semester hours of course work must be taken as a registered master’s degree student at Mines. The student’s committee makes decisions on courses to be taken, transfer credit, and examines the student’s written report. Up to 9 semester hours of graduate courses may be transferred into the degree program, provided that those courses have not been used as credit toward a Bachelor’s degree.

Mines’ Combined Undergraduate / Graduate Degree Program
Students enrolled in Mines’ combined undergraduate/graduate program (meaning uninterrupted registration from the time the student earns a Mines undergraduate degree to the time the student begins a Mines graduate degree) may double count up to six hours of credits which were used in fulfilling the requirements of their undergraduate degree at Mines, towards their graduate program. Any courses that count towards the graduate degree requirements as either “Required Coursework” or “Elective Coursework”, as defined below, may be used for the purposes of double counting at the discretion of the advisor (MS Non-Thesis) or thesis committee (MS Thesis or PhD). These courses must have been passed with a “B-” or better and meet all other University, Department, Division, and Program requirements for graduate credit.

PhD Degree (Applied Chemistry): The program of study for the PhD degree in Applied Chemistry includes coursework, a comprehensive examination, a thesis proposal, research, and the preparation and oral defense of a PhD thesis based on the student’s research.

Coursework. The required courses are:

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</table>
CHGN560  GRADUATE SEMINAR, M.S. (M.S.-level seminar)  1.0
CHGN660  GRADUATE SEMINAR, Ph.D. (Ph.D.-level seminar)  1.0

Total Semester Hrs  14.0

The total hours of course work required for the PhD degree is determined on an individual basis by the student's thesis committee. Up to 24 semester hours of graduate-level course work may be transferred from other institutions toward the PhD degree provided that those courses have not been used by the student toward a Bachelor's degree. Up to 36 hours of credit may be transferred if the student has completed a Master's degree. The student's thesis committee may set additional course requirements and will make decisions on requests for transfer credit.

Seminar requirement. Students should enroll in CHGN560 in the first semester of their degree program. The CHGN560 seminar must be completed no later than the end of the student's second year of graduate studies at Mines. The semester after completion of the CHGN560 seminar, students must enroll in CHGN660. The CHGN660 seminar must include detailed research findings and interpretation of the student’s PhD thesis research and must be presented close to, but before, the student's oral defense of the thesis.

Comprehensive examination. The comprehensive examination comprises a written literature review of the student’s field of research, an oral presentation and defense of the literature review before the student’s thesis committee, and oral answers to questions posed by the thesis committee during the defense. The literature review must be completed prior to the end of the student's second year of graduate studies. A student's thesis committee may, at its discretion, require additional components to the comprehensive examination process.

Thesis proposal. The thesis proposal should include a statement of the hypotheses, goals and objectives of the proposed research, the significance and novelty of the research in the context of previously published studies, a description of methodology and results to date, a timeline with milestones, and a description of how the student has contributed to the creation or direction of the project. The thesis proposal must be orally defended before the student's thesis committee prior to completion of the student's third year of studies.

Geochemistry

Please see the Geochemistry (http://catalog.mines.edu/graduate/programs/interdisciplinaryprograms/geochemistry/) section of this bulletin for more information.

Fields of Research


Geochemistry and biogeochemistry. Microbial and chemical processes in global climate change, biominalization, metal cycling, medical and archeological geochemistry, humic substances.

Inorganic Chemistry. Synthesis, characterization, and applications of metal, metal oxide, and semiconductor nanomaterials.


Physical and Computational Chemistry. Computational chemistry for polymer design, clathrate hydrates, porous media, molecular simulation, energy sciences, biophysical chemistry, rational design of molecular materials, photochemical processes and excited state dynamics, and materials research. Surface-enhanced Raman spectroscopy. Laser Flash Photolysis.


Courses

CHGN502. ADVANCED INORGANIC CHEMISTRY. 3.0 Semester Hrs. (II) Detailed examination of topics such as ligand field theory, reaction mechanisms, chemical bonding, and structure of inorganic compounds. Emphasis is placed on the correlations of the chemical reactions of the elements with periodic trends and reactivities. Prerequisite: none. 3 hours lecture; 3 semester hours.

CHGN503. ADV PHYSICAL CHEMISTRY I. 3.0 Semester Hrs. (II) Quantum chemistry of classical systems. Principles of chemical thermodynamics. Statistical mechanics with statistical calculation of thermodynamic properties. Theories of chemical kinetics. 3 hours lecture; 3 semester hours. Prerequisite: none.

CHGN505. ADVANCED ORGANIC CHEMISTRY. 3.0 Semester Hrs. Detailed discussion of the more important mechanisms of organic reaction. Structural effects and reactivity. The application of reaction mechanisms to synthesis and structure proof. Prerequisite: none. 3 hours lecture; 3 semester hours.

CHGN507. ADVANCED ANALYTICAL CHEMISTRY. 3.0 Semester Hrs. (I) Review of fundamentals of analytical chemistry. Literature of analytical chemistry and statistical treatment of data. Manipulation of real substances; sampling, storage, decomposition or dissolution, and analysis. Detailed treatment of chemical equilibrium as related to precipitation, acid-base, complexation and redox titrations. Potentiometry and UV-visible absorption spectrophotometry. Prerequisite: none. 3 hours lecture; 3 semester hours.

CHGN508. ANALYTICAL SPECTROSCOPY. 3.0 Semester Hrs. (II) Detailed study of classical and modern spectroscopic methods; emphasis on instrumentation and application to analytical chemistry problems. Topics include: UV-visible spectroscopy, infrared spectroscopy, fluorescence and phosphorescence, Raman spectroscopy, arc and spark emission spectroscopy, flame methods, nephelometry and turbidimetry, reflectance methods, Fourier transform methods in spectroscopy, photoacoustic spectroscopy, rapid-scanning spectroscopy. Prerequisite: none. 3 hours lecture; 3 semester hours. Offered alternate years.
CHGN510. CHEMICAL SEPARATIONS. 3.0 Semester Hrs.
(I) Survey of separation methods, thermodynamics of phase equilibria, thermodynamics of liquid-liquid partitioning, various types of chromatography, ion exchange, electrophoresis, zone refining, use of inclusion compounds for separation, application of separation technology for determining physical constants, e.g., stability constants of complexes. Prerequisite: CHGN507. 3 hours lecture; 3 semester hours. Offered alternate years.

CHGN511. APPLIED RADIOCHEMISTRY. 3.0 Semester Hrs.
(II) The Applied Radiochemistry course is designed for those who have a budding interest radiochemistry and its applications. A brief overview of radioactivity and general chemistry will be provided in the first three weeks of the course. Follow-on weeks will feature segments focusing on the radiochemistry in the nuclear fuel cycle, radioisotope production, nuclear forensics and the environment. Prerequisites: CHGN121/CHGN122. 3 hours lecture and discussion; 3 semester hours.

CHGN512. COLLOID AND SURFACE CHEMISTRY. 3.0 Semester Hrs.
Introduction to colloid systems, capillarity, surface tension and contact angle, adsorption from solution, micelles and micro - emulsions, the solid/gas interface, surface analytical techniques, van der Waal forces, electrical properties and colloid stability, some specific colloid systems (clays, foams and emulsions) will be introduced.

CHGN515. CHEMICAL BONDING IN MATERIALS. 3.0 Semester Hrs.
(I) Introduction to chemical bonding theories and calculations and their applications to solids of interest to materials science. The relationship between a material?s properties and the bonding of its atoms will be examined for a variety of materials. Includes an introduction to organic polymers. Computer programs will be used for calculating bonding parameters. Prerequisite: none. 3 hours lecture; 3 semester hours.

CHGN523. SOLID STATE CHEMISTRY. 3.0 Semester Hrs.
(I) Dependence of properties of solids on chemical bonding and structure; principles of crystal growth, crystal imperfections, reactions and diffusion in solids, and the theory of conductors and semiconductors. Prerequisite: none. 3 hours lecture; 3 semester hours. Offered alternate years.

CHGN536. ADVANCED POLYMER SYNTHESIS. 3.0 Semester Hrs.
(II) An advanced course in the synthesis of macromolecules. Various methods of polymerization will be discussed with an emphasis on the specifics concerning the syntheses of different classes of organic and inorganic polymers. Prerequisite: CHGN430, ChEN415, MLGN530. 3 hours lecture, 3 semester hours.

CHGN538. ORGANIC SEMICONDUCTORS: NEW TECHNOLOGIES FOR EMERGING APPLICATIONS. 3.0 Semester Hrs.
(II) Organic Light Emitting Diodes (OLEDs) is a display technology that can be found in many commercial products such as the smartphones and tablets. This technology was on the R&D bench-top just 10 years ago and has now reached high volume manufacturing. Other related technologies like organic photovoltaics (OPV) and organic thin film transistors (OTFT) are now on the heels of commercialization as well. This course will provide an overview on how this meteoric rise from bench-top to commercial products occurred as well as the design, synthesis and uses of conjugated organic small molecules, oligomers and polymers in applications such as OLEDs (for flat panel displays and lighting), OPV, OTFT, and sensors. Additional topics to be covered are factors governing the materials physical properties and structure-property relationship in electronic device applications. The prospect of using low cost printing techniques such as inkjet, screen, and gravure printing in the fabrication of roll-to-roll organic based devices will be discussed. Encapsulation, lifetime and reliability issues will also be presented. Prerequisites: Organic Chemistry 1 & 2 are encouraged. 3 hours lecture; 3 semester hours.

CHGN540. PROFESSIONAL SKILLS FOR CHEMICAL SCIENTISTS. 1.0 Semester Hr.
The goal of this course is to provide students a set of skills that are complementary to their core education. The contents of this course cover a broad range of topics that will provide the participants a perspective on careers in science and the skill sets necessary to be successful in each. These skills are in line with the latest recommendations of the American Chemical Society (ACS) and CSM educational goals. In particular, the 2013 ACS Presidential Commission Report on Graduate Education in the Chemical Sciences presents a platform for educational reform that includes a focus on multi-level (from general public to specialists) and multi-platform communication (formal and informal, written, oral), an understanding of the global chemical enterprise and the career possibilities within each, an understanding of networking and collaboration, etc. 1 hour lecture; 1 semester hour.

CHGN555. POLYMER AND COMPLEX FLUIDS COLLOQUIUM. 1.0 Semester Hr.
Equivalent with BELS555, CBEN555, CHEN555, MLGN555. The Polymer and Complex Fluids Group at the Colorado School of Mines combines expertise in the areas of flow and field based transport, intelligent design and synthesis as well as nanomaterials and nanotechnology. A wide range of research tools employed by the group includes characterization using rheology, scattering, microscopy, microfluidics and separations, synthesis of novel macromolecules as well as theory and simulation involving molecular dynamics and Monte Carlo approaches. The course will provide a mechanism for collaboration between faculty and students in this research area by providing presentations on topics including the expertise of the group and unpublished, ongoing campus research. Prerequisites: none. 1 hour lecture; 1 semester hour. Repeatable for credit to a maximum of 3 hours.

CHGN560. GRADUATE SEMINAR, M.S.. 1.0 Semester Hr.
(I, II) Required for all candidates for the M.S. and Ph.D. degrees in chemistry and geochemistry. M.S. students must register for the course during each semester of residency. Ph.D. students must register each semester until a grade is received satisfying the prerequisites for CHGN560. Presentation of a graded non-thesis seminar and attendance at all departmental seminars are required. Prerequisite: Graduate student status. 1 semester hour.
CHGN580. STRUCTURE OF MATERIALS. 3.0 Semester Hrs.
(I) Application of X-ray diffraction techniques for crystal and molecular structure determination of minerals, inorganic and organometallic compounds. Topics include the heavy atom method, data collection by moving film techniques and by diffractometers, Fourier methods, interpretation of Patterson maps, refinement methods, direct methods. Prerequisite: none. 3 hours lecture; 3 semester hours. Offered alternate years.

CHGN581. ELECTROCHEMISTRY. 3.0 Semester Hrs.
(I) Introduction to theory and practice of electrochemistry. Electrode potentials, reversible and irreversible cells, activity concept. Intermolecular attraction theory, proton transfer theory of acids and bases, mechanisms and fates of electrode reactions. Prerequisite: none. 3 hours lecture; 3 semester hours. Offered alternate years.

CHGN583. PRINCIPLES AND APPLICATIONS OF SURFACE ANALYSIS TECHNIQUES. 3.0 Semester Hrs.
(II) Instrumental techniques for the characterization of surfaces of solid materials; Applications of such techniques to polymers, corrosion, metallurgy, adhesion science, microelectronics. Methods of analysis discussed: x-ray photoelectron spectroscopy (XPS), auger electron spectroscopy (AES), ion scattering spectroscopy (ISS), secondary ion mass spectrometry (SIMS), Rutherford backscattering (RBS), scanning and transmission electron microscopy (SEM, TEM), energy and wavelength dispersive x-ray analysis; principles of these methods, quantification, instrumentation, sample preparation. 3 hours lecture; 3 semester hours. Prerequisite: B.S. in Metallurgy, Chemistry, Chemical Engineering, Physics, or consent of instructor.

CHGN584. FUNDAMENTALS OF CATALYSIS. 3.0 Semester Hrs.
(II) The basic principles involved in the preparation, characterization, testing and theory of heterogeneous and homo geneous catalysts are discussed. Topics include chemisorption, adsorption isotherms, diffusion, surface kinetics, promoters, poisons, catalyst theory and design, acid base catalysis and soluble transition metal complexes. Examples of important industrial applications are given. Prerequisite: CHGN222. 3 hours lecture; 3 semester hours.

CHGN585. CHEMICAL KINETICS. 3.0 Semester Hrs.
(II) Study of kinetic phenomena in chemical systems. Attention devoted to various theoretical approaches. Prerequisite: none. 3 hours lecture; 3 semester hours. Offered alternate years.

CHGN598. SPECIAL TOPICS IN CHEMISTRY. 6.0 Semester Hrs.
(I, II, S) Pilot course or special topics course. Topics chosen from special interests of instructor(s) and student(s). Usually the course is offered only once, but no more than twice for the same course content. Prerequisite: none. Variable credit: 0 to 6 credit hours. Repeatable for credit under different titles.

CHGN699. INDEPENDENT STUDY. 0.5-6 Semester Hr.
(I, II) Individual research or special problem projects supervised by a faculty member, also, when a student and instructor agree on a subject matter, content, and credit hours. Prerequisite: ?Independent Study? form must be completed and submitted to the Registrar. Variable credit: 0.5 to 6 credit hours. Repeatable for credit under different topics/ experience and maximums vary by department. Contact the Department for credit limits toward the degree.

CHGN625. MOLECULAR SIMULATION. 3.0 Semester Hrs.
Principles and practice of modern computer simulation techniques used to understand solids, liquids, and gases. Review of the statistical foundation of thermodynamics followed by indepth discussion of Monte Carlo and Molecular Dynamics techniques. Discussion of intermolecular potentials, extended ensembles, and mathematical algorithms used in molecular simulations. Prerequisites: ChEN509 or equivalent, ChEN610 or equivalent recommended. 3 hours lecture; 3 semester hours.

CHGN660. GRADUATE SEMINAR, Ph.D.. 1.0 Semester Hr.
(I, II) Required of all candidates for the doctoral degree in chemistry or geochemistry. Students must register for this course each semester after completing CHGN560. Presentation of a graded nonthesis seminar and attendance at all department seminars are required. Prerequisite: CHGN560 or equivalent. 1 semester hour.

CHGN698. SPECIAL TOPICS IN CHEMISTRY. 6.0 Semester Hrs.
(I, II, S) Pilot course or special topics course. Topics chosen from special interests of instructor(s) and student(s). Usually the course is offered only once, but no more than twice for the same course content. Prerequisite: none. Variable credit: 0 to 6 credit hours. Repeatable for credit under different titles.

CHGN699. INDEPENDENT STUDY. 0.5-6 Semester Hr.
(I, II, S) Individual research or special problem projects supervised by a faculty member, also, when a student and instructor agree on a subject matter, content, and credit hours. Prerequisite: ?Independent Study? form must be completed and submitted to the Registrar. Variable credit: 0.5 to 6 credit hours. Repeatable for credit under different topics/ experience and maximums vary by department. Contact the Department for credit limits toward the degree.

Professors
Mark E. Eberhart
Thomas Gennett, Department Head
Richard C. Holz
Mark P. Jensen, Grandey University Chair in Nuclear Science & Engineering
Daniel M. Knauss
Matthew C. Posewitz
James F. Ranville
Ryan M. Richards
Alan S. Sellinger
Bettina M. Voelker
Kim R. Williams
David T. Wu
Associate Professors
Judith Klein-Seetharaman
Jenifer C. Shafer
Brian G. Trewyn

Assistant Professors
Dylan Domaille
C. Michael McGuirk
Christine Morrison
Svitlana Pylypenko
Shubham Vyas

Teaching Professors
Renee L. Falconer, Assistant Department Head
Mark R. Seger

Teaching Associate Professors
Allison G. Caster
Angela Sower

Teaching Assistant Professors
Amanda Jameer
Jonathan Miorelli

Research Assistant Professors
Jessica Jackson
Yuan Yang

Joint Appointees
Michael Guarnieri
Jesse Hensley
Seonah Kim
Calvin Mukarakate
Bryan Pivovar
David Robichaud
Daniel Ruddy
Robert S. Rundburg
Derek Vardon

Affiliated Faculty
Gayle Bentley
Joseph Meyer
Kathleen Smith

Professor Emeriti
Scott W. Cowley
Stephen R. Daniel
Dean W. Dickerhoof
Kenneth W. Edwards
Ronald W. Klusman
Donald Langmuir
Donald L. Macalady
Patrick MacCarthy
Michael J. Pavelich
E. Craig Simmons
Kent J. Voorhees
Thomas R. Wildeman
John T. Williams