

# 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.

## 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:

CHGN502	ADVANCED INORGANIC CHEMISTRY	3.0
CHGN503	ADV PHYSICAL CHEMISTRY I	3.0
CHGN505	ADVANCED ORGANIC CHEMISTRY	3.0
CHGN507	ADVANCED ANALYTICAL CHEMISTRY	3.0
CHGN560	GRADUATE SEMINAR, M.S. (M.S.-level seminar)	1.0

Students should enroll in CHGN560 in the first semester of their degree program. A minimum of 36 credits, including at least 18 credits of course work, is required. At least 15 of the required 18 credits of course work must be taken in the Department of Chemistry at Mines. The total hours of course work required are determined on an individual basis by the student's thesis committee.

**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 credits:

Course work	24.0
Independent study	6.0
<b>Total Semester Hrs</b>	<b>30.0</b>

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. As part of the 24 credits of required coursework, students must pass CHGN560 (1 credit) as well as three of the four core courses (CHGN502, CHGN503, CHGN505, CHGN507; 3 credits each).

CHGN502	ADVANCED INORGANIC CHEMISTRY	3.0
CHGN503	ADV PHYSICAL CHEMISTRY I	3.0
CHGN505	ADVANCED ORGANIC CHEMISTRY	3.0
CHGN507	ADVANCED ANALYTICAL CHEMISTRY	3.0
CHGN560	GRADUATE SEMINAR, M.S. (M.S.-level seminar)	1.0

Students should enroll in CHGN560 in the first semester of their degree program. At least 21 of the required 30 credits 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 and oral presentation resulting from the independent study. Up to 9 credits 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 may double count up to six credits of graduate coursework to fulfill requirements of both their undergraduate and graduate degree programs. These courses must have been passed with "B-" or better, not be substitutes for required coursework, and meet all other University, Department, and Program requirements for graduate credit.

Students are advised to consult with their undergraduate and graduate advisors for appropriate courses to double count upon admission to the combined program.

## 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:

CHGN502	ADVANCED INORGANIC CHEMISTRY	3.0
CHGN503	ADV PHYSICAL CHEMISTRY I	3.0
CHGN505	ADVANCED ORGANIC CHEMISTRY	3.0
CHGN507	ADVANCED ANALYTICAL CHEMISTRY	3.0
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**

PhD students must receive at minimum a B in required core classes; students who receive a B- or lower need to demonstrate subject competency to continue in the PhD program. At least 18 credits of course work are required for the PhD degree; the total hours of course work required are determined on an individual basis by the student's thesis committee. Up to 24 credits 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 credits 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 section of this bulletin for more information.

## Courses

### CHGN502. ADVANCED INORGANIC CHEMISTRY. 3.0 Semester Hrs.

Detailed examination of concepts such as molecular symmetry, group theory, molecular orbital theory, ligand field theory, and crystal field theory. Additional topics include spectroscopy, inorganic reaction mechanisms, and organometallic chemistry.

### 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.

### CHGN509. BIOLOGICAL INORGANIC CHEMISTRY. 3.0 Semester Hrs.

This course starts with a short introduction to inorganic chemistry and biology. The course then focuses on core bioinorganic chemistry topics, including metalloprotein structure and function; characterization of bioinorganic systems; metal assimilation, metabolism, and homeostasis; and metals in medicine. We also briefly cover special topics, such as metallo-endocrinology, extremophiles, biomineralization, and supramolecular bioinorganic chemistry. We investigate recent advances in the field of bioinorganic chemistry, introduce many leading scientists in the field, and explore scientific literature. Students are assessed through two open-resource, take-home exams (midterm and final) covering course material. Students also explore a topic of their choice through a class presentation and a writing assignment. There are no formal prerequisites for the class; however, students will benefit from having taken at least one of the following courses: organic chemistry, inorganic chemistry, or biochemistry.

### CHGN510. CHEMICAL SEPARATIONS. 3.0 Semester Hrs.

(II) 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. 3 hours lecture and discussion; 3 semester hours. Prerequisite: CHGN 122 or CHGN 125.

### 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.

**CHGN535. PHYSICAL BIOCHEMISTRY. 3.0 Semester Hrs.**

Apply physical chemical principles to understand property-function relationships of biochemical molecules, and investigate biochemical instrumentation and quantitative analyses common to biochemistry. Methods discussed include light/fluorescence microscopy, biomolecular structure determination, i.e., X-ray crystallography, cryo-electron microscopy and NMR, scattering techniques, biomolecular motors, and more. Prerequisite: CHGN 428 + CHGN 209 or equivalent (CBEN 210 or BIOL 301) Co-requisite: N/A.

**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. 3 hours lecture, 3 semester hours Prerequisite: CHGN 430, CBEN 415, MLGN 530.

**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 CBEN555,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 CHGN660. 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.**

(II) 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. Interionic 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 homogeneous 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.

**CHGN599. 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.

**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 in-depth discussion of Monte Carlo and Molecular Dynamics techniques. Discussion of intermolecular potentials, extended ensembles, and mathematical algorithms used in molecular simulations. 3 hours lecture; 3 semester hours. Prerequisite: CBEN 509 or equivalent, and recommend CBEN 610 or equivalent.

**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.

**CHGN707. GRADUATE THESIS / DISSERTATION RESEARCH CREDIT. 1-15 Semester Hr.**

(I, II, S) Research credit hours required for completion of a Masters-level thesis or Doctoral dissertation. Research must be carried out under the direct supervision of the student's faculty advisor. Variable class and semester hours. Repeatable for credit.

## Professors

Thomas Albrecht-Schönzart, Distinguished Professor

Thomas Gennett, Department Head

Richard C. Holz, Provost

Mark P. Jensen, Grandey University Chair in Nuclear Science & Engineering

Daniel M. Knauss, Associate Dean of Energy and Materials

Matthew C. Posewitz

James F. Ranville

Ryan M. Richards

Alan S. Sellinger

Jenifer C. Shafer

Bettina M. Voelker

David T. Wu

## Associate Professors

Svitlana Pylypenko

Brian G. Trewyn

Shubham Vyas

## Assistant Professors

Dylan Domaille

Annalise Maughan

C. Michael McGuirk

Christine Morrison

## Teaching Professors

Renee L. Falconer, Assistant Department Head

Angela Sower

## Teaching Assistant Professors

Christian Beren

Amanda Jameer

Kara Metzger

Jonathan Miorelli

Michael J. Pavelich

Mark R. Seger

E. Craig Simmons

Kent J. Voorhees

Thomas R. Wildeman

## Research Professors

Mark E. Eberhart

Kim R. Williams

## Research Assistant Professors

Shane Galley

Jessica Jackson

Yuan Yang

## Joint Appointees

Matthew Beard

Todd Deutsch

Jesse Hensley

Justin Johnson

Calvin Mukarakate

Bryan Pivovar

David Robichaud

Daniel Ruddy

## Affiliated Faculty

Samuel Bryan

Stosh Kozimor

Lieve Laurens

Joseph Meyer

Kathleen Smith

Angela Stelson

## Professor Emeriti

Scott W. Cowley

Dean W. Dickerhoof

Mark E. Eberhart

Ronald W. Klusman

Donald Langmuir

Donald L. Macalady

Patrick MacCarthy