

DOCTORATE IN PHILOSOPHY CHEMISTRY AND SPECIALIZATION CHEMICAL AND ENVIRONMENTAL TOXICOLOGY

Summary

- Degree offered: Doctorate in Philosophy (PhD)
- Registration status option: Full-time
- Language of instruction:
 - French
 - English

Note: Most of the courses in this program are offered in English.

- Primary program: PhD in Chemistry
- Collaborative specialization: Chemical and Environmental Toxicology
- Program option (expected duration of the program):
 - with thesis (12 full-time terms; 48 consecutive months)
- Academic units: Faculty of Science (<http://science.uottawa.ca/>), Department of Chemistry and Biomolecular Sciences (<http://science.uottawa.ca/chemistry/>), Ottawa-Carleton Chemistry Institute.

Program Description

Ottawa-Carleton Joint Program

Established in 1981, the Ottawa-Carleton Chemistry Institute (OCCI) combines the research strengths of the University of Ottawa and Carleton University. The institute offers graduate programs leading to the master's (MSc) and doctoral (PhD) degrees in Chemistry.

Research facilities are shared between the two campuses. Students have access to the professors, courses and facilities at both universities; however, they must enroll at the "home university" of the thesis supervisor.

The Institute is a participating unit in the collaborative program in science, society and policy at the master's level and in chemical and environmental toxicology at the master's and doctoral levels.

Collaborative Program Description

Toxicology is the study of effects of toxic substances on living systems. These toxic substances can either be organic or inorganic, synthetic or natural materials. Environmental toxicology further extends to aspects of chemical transport, fate, persistence and biological accumulation of toxic substances and their effects at the population and community levels. While individual researchers usually specialize in a particular area, toxicologists today must be able to appreciate significant research in other fields and therefore require an understanding of the basic principles of other disciplines. To meet this challenge the University of Ottawa and Carleton University offer a joint collaborative program leading to a master of science or a PhD degree with specialization in chemical and environmental toxicology.

This Ottawa-Carleton collaborative program in Chemical and Environmental Toxicology is intended to augment the research and training available to students through the individual supporting institutes.

Main Areas of Research

- Inorganic chemistry
- Organic chemistry
- Theoretical chemistry
- Biological chemistry
- Analytical chemistry
- Physical chemistry

Other Programs Offered Within the Same Discipline or in a Related Area

- Master of Science Chemistry (MSc)
- Master of Science Chemistry Specialization in Science, Society and Policy (MSc)
- Master of Science Chemistry Specialization in Chemical and Environmental Toxicology (MSc)
- Doctorate in Philosophy Chemistry (PhD)

Fees and Funding

- Program fees:

The estimated amount for university fees (<https://www.uottawa.ca/university-fees/>) associated with this program are available under the section Finance your studies (<http://www.uottawa.ca/graduate-studies/programs-admission/finance-studies/>).

International students enrolled in a French-language program of study may be eligible for a differential tuition fee exemption (<https://www.uottawa.ca/university-fees/differential-tuition-fee-exemption/>).

- To learn about possibilities for financing your graduate studies, consult the Awards and financial support (<https://www.uottawa.ca/graduate-studies/students/awards/>) section.

Notes

- Programs are governed by the academic regulations (<https://www.uottawa.ca/about-us/leadership-governance/policies-regulations/>) in effect for graduate studies at each of the two universities.
- In accordance with the University of Ottawa regulation, students have the right to complete their assignments, examinations, research papers, and theses in French or in English.
- Research activities can be conducted either in English, French or both, depending on the language used by the professor and the members of his or her research group.

Program Contact Information

Graduate Studies Office, Faculty of Science (<https://science.uottawa.ca/en/faculty-services/graduate-studies/>)

30 Marie-Curie Street, Gendron Hall, Room 181

Ottawa, Ontario, Canada

K1N 6N5

Tel.: 613-562-5800 x3145

Email: gradsci@uOttawa.ca

Twitter | Faculty of Science (<https://twitter.com/uOttawaScience/?lang=en>)

Facebook | Faculty of Science (<https://www.facebook.com/uOttawaScience/>)

Admission Requirements

For the most accurate and up to date information on application deadlines, language tests and other admission requirements, please visit the specific requirements (<https://www.uottawa.ca/graduate-studies/programs-admission/apply/specific-requirements/>) webpage.

To be eligible, candidates must:

- Have a master's degree in Chemistry (or equivalent) with a minimum admission average of 75% (B+).

Note: International candidates must check the admission equivalencies (<https://www.uottawa.ca/graduate-studies/international/study-uottawa/admission-equivalencies/>) for the diploma they received in their country of origin.

- Demonstrate high academic achievement, as indicated in official transcripts, research reports, abstracts or any other documents demonstrating research skills.
- Meet the funding requirements.

Note: International students must provide proof of financial support: i.e., a stipend provided by a supervisor as well as a combination of awards and/or trust funds.

- Identify at least one professor who is willing to supervise your research and thesis.
 - We recommend that you contact potential thesis supervisors as soon as possible.
 - To register, you need to have been accepted by a thesis supervisor.
 - The supervisor's name is required at the time of application.
 - The choice of supervisor will determine the primary campus location of the student. It will also determine which university awards the degree.
- Be sponsored into the collaborative specialization by a faculty member of the collaborative program, normally the thesis supervisor, who must be appointed, cross-appointed or stand as an adjunct at the primary program.
- Meet the following additional requirements:
 - Complete a relevant introductory course in toxicology, either:
 - Prior to admission to the collaborative program in chemical and environmental toxicology; or
 - While enrolled in the program by taking one of the two introductory courses (TOX 8156 or TOX 9104).

Language Requirements

Applicants must be able to understand, write and fluently speak the language of instruction (French or English) in the program to which they are applying. Proof of linguistic proficiency may be required.

Applicants whose first language is neither French nor English must provide proof of proficiency in the language of instruction.

Note: Candidates are responsible for any fees associated with the language tests.

Notes

- The admission requirements listed above are minimum requirements and do not guarantee admission to the program.
- Admissions are governed by the academic regulations (<https://www.uottawa.ca/about-us/leadership-governance/policies-regulations/>) in effect for graduate studies and the general regulations of the Ottawa-Carleton Institute for Chemistry (OCIC)
- Candidates must apply to the primary program and indicate in their application for admission to the PhD program in Chemistry that they wish to be accepted into the collaborative-specialization in Chemical and Environmental Toxicology. Applications for admission may also be submitted upon acceptance into the primary PhD program at the University of Ottawa. To be admitted to the collaborative program, candidates must also be accepted in the primary program.

Fast-Track from Master's to PhD

Students enrolled in the master's program in Chemistry at the University of Ottawa may be eligible to fast-track directly into the doctoral program without writing a master's thesis, provided the following conditions are met:

- Completion of four graduate courses (6 units) with a grade of A- or better in each.
- Satisfactory progress in the research program.

- Written recommendation by the supervisor and the advisory committee.
- Approval by the graduate studies committee.

Notes:

- The transfer must take place within sixteen months of initial enrollment in the master's.
- The minimal admission average requirements for the doctoral program must also be met.
- Students in the Accelerated Stream are not eligible to fast-track to the PhD program.

Program Requirements

Doctorate with Collaborative Specialization

Requirements for this program have been modified. Please consult the 2018-2019 calendars (<https://catalogue.uottawa.ca/en/archives/>) for the previous requirements.

The Department may require students to take additional courses, depending on their backgrounds. The course units completed for the specialization count also towards the primary degree.

Students must meet the following requirements for the doctorate with collaborative specialization:

Compulsory Courses:

3 course units from:	3 Units
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TOX 8156	Principles of Toxicology
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TOX 9104	Ecotoxicology
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3 optional course units in chemistry (CHM) at the graduate level ¹	3 Units
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Seminars: ²

CHM 8257	Seminar II	1 Unit
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TOX 9105	Seminar in Toxicology ³	3 Units
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Comprehensive Examination:

CHM 9998	Ph.D. Comprehensive ⁴
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Thesis Proposal:

CHM 8958	Research Proposal ⁵
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Thesis:

THD 9999	Doctoral Thesis ^{6, 7}
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Note(s)**1**

The optional course units may also be selected from related disciplines approved by the Department of Chemistry.

2

The seminar courses involve the presentation of a seminar and the regular attendance at the departmental seminar series.

3

Students who completed the seminar course TOX 9105 for the master's specialization are exempted from this requirement.

4

The comprehensive examination must be completed within twelve months of initial enrollment in the program.

5

The thesis proposal must be completed before the end of the sixth term of enrollment in the program.

6

Presentation and defense of a thesis in toxicology based on an original research carried out under the supervision of a faculty member participating in the chemical and environmental toxicology collaborative program.

7

Students are responsible for ensuring they have met all of the thesis requirements (<http://www.uottawa.ca/graduate-studies/students/theses/>).

Transfer from Master's to PhD

Following the transfer, all of the requirements of the doctoral program must be met: a total number of twelve units of graduate coursework (MSc+PhD); the seminar (CHM 8257); the comprehensive examination (CHM 9998); the thesis proposal (CHM 8958) and the thesis (THD 9999).

Minimum Requirements

The passing grade in all courses is B.

Research

Research at the University of Ottawa

Located in the heart of Canada's capital, a few steps away from Parliament Hill, the University of Ottawa ranks among Canada's top 10 research universities. Our research is founded on excellence, relevance and impact and is conducted in a spirit of equity, diversity and inclusion.

Our research community thrives in four strategic areas:

- Creating a sustainable environment
- Advancing just societies
- Shaping the digital world
- Enabling lifelong health and wellness

From advancing healthcare solutions to tackling global challenges like climate change, the University of Ottawa's researchers are at the forefront of innovation, making significant contributions to society and beyond.

Research at the Faculty of Science

The Faculty of Science has become a true centre of excellence in research through its world-class professors as well as its programs and infrastructure in Biology, Chemistry, Earth Sciences, Mathematics and Statistics, and Physics.

The research accomplished by its 140 internationally recognized professors, its approximately 400 graduate students and its dozens of postdoctoral researchers and visiting scientists has positioned the Faculty of Science as one of the most research intensive science faculties in Canada. Our professors have received many international and national awards including three NSERC Gerhard Herzberg Gold Medal winners and numerous Fellows of the Royal Society of Canada.

The Faculty of Science, through its strategic use of infrastructure programs, hosts world-class Core Facilities and is at the leading edge for the study of Catalysis, Experimental and Computational Chemistry, Environmental Toxins, Nuclear Magnetic Resonance, Isotope Analysis,

Molecular Biology and Genomics, X-Ray Spectrometry/Diffractometry, Geochemistry, Mass Spectrometry, Physiology and Genetics of Aquatic Organisms, and Photonics. The Faculty is also associated with the Fields Institute for research in mathematical science and the Centre de recherche mathématiques (CRM) at the Université de Montréal, providing a unique setting for mathematical research.

For more information, refer to the list of faculty members and their research fields on **Uniweb**.

IMPORTANT: Candidates and students looking for professors to supervise their thesis or research project can also consult the website of the faculty or department (<https://www.uottawa.ca/study/graduate-studies/academic-unit-contact-information/>) of their program of choice. Uniweb does not list all professors authorized to supervise research projects at the University of Ottawa.

Courses

Not all of the listed courses are given each year. The course is offered in the language in which it is described.

A 3-unit course at the University of Ottawa is equivalent to a 0.5-unit course at Carleton University.

CHM 5105 Radiochemistry (3 units)

A study of nuclear stability and decay; chemical studies of nuclear phenomena. Application of radioactivity.

Course Component: Lecture

Permission of the Department is required.

CHM 5108 Surface Chemistry and Nanostructures (3 units)

Surface structure, thermodynamics and kinetics, specifically regarding adsorption/desorption and high vacuum models. Nanoscale structures and their formation, reactivity and characterization. Thin films, carbon nanotubes, self-assembled monolayers and supramolecular aggregates. This course is equivalent to CHEM 5108 at Carleton University

Course Component: Lecture

CHM 5109 Advanced Applications in Mass Spectrometry (3 units)

Detailed breakdown of the physical, electrical and chemical operation of mass spectrometers. Applications in MS ranging from the analysis of small molecules to large biological macromolecules. Descriptions of the use of mass spectrometry in industry as well as commercial opportunities in the field. This course is equivalent to CHEM 5109 at Carleton University.

Course Component: Lecture

CHM 5206 Physical Methods of Nanotechnology (3 units)

An overview of methods used in nanotechnology. Principles of scanning probe techniques ranging from surface physics to biology. State of the art methods to create nanostructures for future applications in areas such as nanolithography, nanoelectronics, nano-optics, data storage and bio-analytical nanosystems. This course is equivalent to CHEM 5206 at Carleton University.

Course Component: Lecture

CHM 5207 Macromolecular Nanotechnology (1.5 unit)

Fundamentals of synthetic macromolecules related to nanoscale phenomena. Challenges and opportunities associated with polymers on the nanoscale. Topics include molecular recognition, self-assembled nanostructures, functional nanomaterials, amphiphilic architectures, nanocomposites, and nanomachines. Applications to sensing, drug delivery, and polymer based devices. This course is equivalent to CHEM 5207 at Carleton University.

Course Component: Lecture

CHM 5208 Bio Macromolecular Nanotechnology (1.5 unit)

Fundamentals of biological macromolecules related to nanoscale phenomena. Challenges and opportunities associated with natural polymers on the nanoscale. Topics include molecular recognition, self-assembled nanostructures, scaffolds and templates, functional nanomaterials, amphiphilic architectures, nanocomposites, and nanomachines. Applications to sensing, biomaterials, drug delivery, and devices. This course is equivalent to CHEM 5208 at Carleton University.

Course Component: Lecture

CHM 5606 Environmental Chemistry and Toxicology (1.5 crédit)

Overview of environmental chemistry and toxicology principles including chemical sources, fate, and effects in the environment. Examining organic reactions occurring in abiotic environments and biological systems, and study aspects of toxicant disposition and biotransformation. Emphasis on contemporary problems in human health and the environment. This course is equivalent to CHEM 5606 at Carleton University

Volet : Cours magistral

CHM 8104 Scientific Data Processing and Evaluation (3 units)

Optimization of scientific measurements, calibration, uni-variate and multi-variate analysis of scientific data, 'intelligent' spreadsheets for scientific data processing and presentation, noise reduction using spreadsheets, correction for signal drifts; examples from chemistry, spectroscopy and other scientific disciplines. This course is equivalent to CHEM 5904 at Carleton University.

Course Component: Lecture

CHM 8126 Bioorganic Chemistry (3 units)

Overview of recent developments in the mechanistic understanding of selected enzyme-catalyzed reactions. Topics include Cytochrome P450, methane monooxygenase, biotin and lipoic acid biosynthesis, methyl transfer, Vitamin B12, lipoxygenase, prostaglandin synthase; etc. Emphasis will be placed on biotransformations which are relatively poorly understood from a mechanistic point of view. This course is equivalent to CHEM 5303 at Carleton University.

Course Component: Lecture

CHM 8134 Spectroscopy for Organic Chemists (3 units)

Analysis of proton NMR spectra. Fourier transform ¹³C NMR, strategies for structure elucidation, relaxation times, two-dimensional NMR. Aspects of mass spectrometry. This course is equivalent to CHEM 5407 at Carleton University.

Course Component: Lecture

CHM 8150 Special Topics in Molecular Spectroscopy (3 units)

Topics of current interest in molecular spectroscopy. In past years, the following areas have been covered: electronic spectra of diatomic and triatomic molecules and their interpretation using molecular orbital diagrams; Raman and resonance Raman spectroscopy; symmetry aspects of vibrational and electronic levels of ions and molecules in solids in the presence of weak and strong resonant laser radiation. This course is equivalent to CHEM 5009 at Carleton University.

Course Component: Lecture

CHM 8158 Directed Special Studies (3 units)

Under unusual circumstances and with the recommendation of the research supervisor, it is possible to engage in a directed study on a topic of particular value to the student. This may also be used for unit if there are insufficient course offerings in a particular field of chemistry. This course is equivalent to CHEM 5900 at Carleton University.

Course Component: Lecture

CHM 8164 Organic Polymer Chemistry (3 units)

Basic principles of industrial and synthetic polymers. Polymerization and polymer characterization. Selected topics to cover some important polymers with emphasis on the synthesis, commodity plastics, engineering thermoplastics and specialty polymers. Students should have a basic knowledge of organic reaction mechanisms and stereochemistry. This course is equivalent to CHEM 5406 at Carleton University.

Course Component: Lecture

Prerequisites: CHM 3120, CHM 4120, CHM 4125, equivalent. or A basic knowledge of organic reaction mechanisms and stereochemistry.

CHM 8165 Advanced Protein Engineering (3 units)

Overview of recent developments in the conception and design of proteins with novel structures and functions. Topics include rational and computational design, ancestral protein reconstruction, and directed evolution of proteins.

Course Component: Lecture

CHM 8173 Introduction to Molecular Simulation and Statistical Mechanics (Part A) (1.5 unit)

A practical introduction to modern molecular simulation techniques widely used as tools in chemical research. Classical molecular dynamics and Monte Carlo simulations methods are discussed. The necessary statistical mechanics required to understand and properly interpret the molecular simulations and link the results to measured bulk properties are introduced. An introduction to modern scientific computing environments and the Linux operating system is also provided. This course is equivalent to CHEM 5114 at Carleton University.

Course Component: Lecture

CHM 8174 Stereoselective Synthesis (1.5 unit)

Fundamentals of stereoselective synthesis and catalysis, including conformational analysis, substrate and catalyst control. Includes the use of allylic, chiral auxiliaries, directed reactions and chiral catalysts. This course is equivalent to CHM 5113 at Carleton University.

Course Component: Lecture

CHM 8175 Introduction to Molecular Simulation and Statistical Mechanics (Part B) (1.5 unit)

A practical introduction to modern molecular simulation techniques widely used as tools in chemical research. Classical molecular dynamics and Monte Carlo simulations methods are discussed. The necessary statistical mechanics required to understand and properly interpret the molecular simulations and link the results to measured bulk properties are introduced. An introduction to modern scientific computing environments and the Linux operating system is also provided. This course is equivalent to CHEM 5115 at Carleton University.

Course Component: Lecture

CHM 8176 Chemistry Education and Chemistry Education Research (1.5 unit)

Overview of key areas of chemistry education, including theories of learning, aligning intended outcomes with course activities and assessment, and troublesome areas of learning and teaching in chemistry. Key educational research areas are addressed, including types evidence, research methods, and central publications. This course is equivalent to CHEM 5110 at Carleton University

Course Component: Lecture

CHM 8180 Directed Special Studies (1.5 unit)

Under unusual circumstances and with the recommendation of the research supervisor, it is possible to engage in a directing study on a topic of particular value to the student. This may also be used for unit if there are insufficient course offerings in a particular field of chemistry. This course is equivalent to CHEM 5900 at Carleton University.

Course Component: Lecture

CHM 8181 Chemical Physics of Electron-Molecule Collisions (3 units)

Basic classical scattering theory and quantum mechanical scattering theory. Experimental aspects, such as electron optics, electron gun fundamentals, energy analyzers and electron detectors. Applications to the understanding of the chemistry of materials. This course is equivalent to CHEM 5101 at Carleton University.

Course Component: Lecture

CHM 8256 Seminar I (1 unit)

A seminar course in which students are required to present a seminar on a topic not related to their research project. In addition, students are required to attend the seminar of their fellow classmates and actively participate in the discussion following the seminar. This course is equivalent to CHEM 5801 at Carleton University.

Course Component: Seminar

CHM 8257 Seminar II (1 unit)

A seminar course in which students are required to present a seminar on their Ph.D research project. In addition, students are required to attend the seminars of the fellow classmates and departmental seminars, and actively participate in the discussion. This course is equivalent to CHEM 5802 at Carleton University.

Course Component: Seminar

CHM 8301 Analytical Mass Spectrometry (1.5 unit)

The principles of ion sources and mass spectrometers will be described, together with their applications to problems in chemistry and biochemistry. Introduction to the chemistry gaseous ions. Ion optics. Special emphasis on interpreting mass spectra. This course is equivalent to CHEM 5001 at Carleton University.

Course Component: Lecture

CHM 8302 Advanced Topics in Inorganic Chemistry (1.5 unit)

Topics of current interest in inorganic chemistry. Variable content from year to year. This course is equivalent to CHEM 5902 at Carleton University.

Course Component: Lecture

CHM 8303 Descriptive Organometallic Chemistry (1.5 unit)

Review of basic concepts of M-C bonds and of the preparation and reactivity of transition and non-transition metal organometallic species. Brief discussion of the most important catalytic processes (e.g. Ziegler-Natta, Fisher-Tropsch, catalytic hydrogenation and hydroformylation). This course is equivalent to CHEM 5204 at Carleton University.

Course Component: Lecture

CHM 8304 Advanced Topics in Organic Chemistry (1.5 unit)

Topics of current interest in organic chemistry. Variable content from year to year. This course is equivalent to CHEM 5901 at Carleton University.

Course Component: Lecture

CHM 8308 Multinuclear Magnetic Resonance Spectroscopy (1.5 unit)

Principles of Nuclear Magnetic Resonance (NMR). Study of NMR parameters: chemical shift, spin-spin coupling, electric quadrupole coupling, spin-spin and spin-lattice relaxation rates. NMR and the periodic table. Dynamic NMR. Applications in chemistry and biochemistry. Fourier Transform technique. Pulse sequences. Basic principles and applications of two-dimensional NMR. This course is equivalent to CHEM 5002 at Carleton University.

Course Component: Lecture

CHM 8309 Advanced Topics in Physical (1.5 unit)

Topics of current interest in physical/theoretical chemistry. Variable content from year to year. This course is equivalent to CHEM 5903 at Carleton University.

Course Component: Lecture

CHM 8310 Introduction to Photochemistry (1.5 unit)

Basic principles of photochemistry including selection rules, energy transfer processes and the properties of excited state reactions. Lasers and their applications to measurements of the dynamics of elementary reactions. This course is equivalent to CHEM 5007 at Carleton University.

Course Component: Lecture

CHM 8311 Advanced and Applied Photochemistry (1.5 unit)

Photochemical reactions of small molecules and their relationship to atmospheric chemistry. Production and detection of reactive species. Photolysis. Multiphoton absorption. This course is equivalent to CHEM 5008 at Carleton University.

Course Component: Lecture

Prerequisite: CHM 8310

CHM 8314 Surface Chemistry Aspects of Electrochemical Science (1.5 unit)

Introduction to electrode processes and electrolysis. Potential differences at interfaces. Characterization of the electrical double layer. Dipole orientation effects, charge-transfer in adsorbed layers, electrochemical origins of surface science concepts. Theory of electron transfer, electrode kinetics, electrocatalysis. This course is equivalent to CHEM 5504 at Carleton University.

Course Component: Lecture

CHM 8315 Electrochemical Surface Science (1.5 unit)

Introduction to advanced in-situ techniques in electrochemistry: Scanning probe microscopy, Raman, infrared and laser spectroscopy. This course is equivalent to CHEM 5505 at Carleton University.

Course Component: Lecture

Prerequisites: CHM 8314, CHM 8714

CHM 8316 Surface Chemistry (1.5 unit)

Adsorption phenomena and isotherms, surface areas of solids. Modern techniques in surface chemistry and surface science such as electron diffraction, Auger electron spectroscopy, photoelectron spectroscopy, electron energy loss spectroscopy, infrared and Raman spectroscopy. Current new techniques. This course is equivalent to CHEM 5506 at Carleton University.

Course Component: Lecture

CHM 8319 Total Syntheses (1.5 unit)

Discussion on philosophy and strategy development for complex syntheses, along with modern reagents and reactions that have shortened classical routes and lead to more efficient and atom economy. This course is equivalent to CHEM 5403 at Carleton University.

Course Component: Lecture

CHM 8320 Pericyclic and Stereoelectronic Effects (1.5 unit)

Pericyclic reactions, facial selectivity, stereoelectronic effects in carbohydrates and related acetal cleavage. Applications to complex synthetic problems. This course is equivalent to CHEM 5405 at Carleton University.

Course Component: Lecture

CHM 8321 Solid State Chemistry (1.5 unit)

Thermodynamic and kinetic aspects of solid state synthesis. Characterization of solids. Chemical and physical properties of solids that may include aspects of intercalation reactions, ionic conductors, glasses, electronic, magnetic optical and physical/mechanical properties. This course is equivalent to CHEM 5201 at Carleton University.

Course Component: Lecture

CHM 8322 Topics in Coordination Chemistry (1.5 unit)

Brief introduction to basic concepts in coordination chemistry. Topics to include the following: carbon dioxide fixation, dinitrogen fixation, activation, olefin metathesis, nature of the M-M bond. This course is equivalent to CHEM 5203 at Carleton University.

Course Component: Lecture

CHM 8323 Quantum Mechanical Methods - Theory (1.5 unit)

Examination of the theory behind quantum mechanical methods (HF, MP2, CI, DFT). Semi-empirical. This course is equivalent to CHEM 5600 at Carleton University.

Course Component: Lecture

CHM 8324 Quantum Mechanical Methods - Applications (1.5 unit)

Practical applications of methods taught in CHM 8323 such as thermochemistry, reaction pathway modeling, structure predictions. This course is equivalent to CHEM 5601 at Carleton University.

Course Component: Lecture

Prerequisite: CHM 8323 or CHM 8723

CHM 8325 Solid State Nmr Spectroscopy (1.5 unit)

Brief introduction to solid state NMR spectroscopy. Topics include dipolar coupling interactions, chemical shielding anisotropy, the quadrupolar interaction and averaging techniques such as magic angle spinning. This course is equivalent to CHEM 5003 at Carleton University.

Course Component: Lecture

CHM 8326 Nmr Spectroscopy (1.5 unit)

Advanced NMR techniques for both proton and carbon spectra, various decoupling and related experiments. Interpretation of NIOSY, COSY and related data. This course is equivalent to CHEM 5004 at Carleton University.

Course Component: Lecture

CHM 8327 Physical Organic Chemistry (1.5 unit)

Transition state theory, experimental kinetics and thermodynamics, isotope effects, Linear Free Energy Relationships (LFERs), catalysis and Reaction Profile Kinetic Analysis (RPKA). This course is equivalent to CHEM 5005 at Carleton University.

Course Component: Lecture

CHM 8328 Applications of Organometallic Chemistry to Synthesis (1.5 unit)

Study of organometallic methods, many of which have become catalytic and involve metals such as Cu, Pd, Pt, Mo, Cr, Ru. Various applications to be discussed including Stille coupling, Heck reaction, ring closing metathesis. This course is equivalent to CHEM 5401 at Carleton University.

Course Component: Lecture

CHM 8329 Medicinal Chemistry (1.5 unit)

Preparation of drugs, their mode of action, their use in treating of disease. Evolution of medicine due to chemistry. Discussion of metabolic pathways and their modification to control and/or circumvent disease. This course is equivalent to CHEM 5402 at Carleton University.

Course Component: Lecture

CHM 8330 Heterocyclic Chemistry (1.5 unit)

Properties of heterocycles. Synthesis and reactivity of heterocyclic systems, with examples relevant to the synthesis of pharmaceuticals and natural products. Includes metal-catalysed reactions. This course is equivalent to CHEM 5120 at Carleton University.

Course Component: Lecture

CHM 8331 Physical Chemistry of Biological Macromolecules (1.5 unit)

Focus on how the application of physical techniques, normally applied to small molecules, can be used to study macromolecular structure and function of DNA and proteins. Examples of applications to include: kinetics, electrochemistry, equilibria phenomena (thermodynamics). This course is equivalent to CHEM 5300 at Carleton University.

Course Component: Lecture

CHM 8332 Electrochemical Phenomena in Biological Systems (1.5 unit)

Description of theory accounting for the generation of membrane potentials. Application to the generation of nerve impulses. This course is equivalent to CHEM 5301 at Carleton University.

Course Component: Lecture

CHM 8333 Surface Phenomena in Biological Systems (1.5 unit)

Description of theory of surface tension phenomena in aqueous systems. Discussion of effects of cell and macromolecular structures in biological systems. This course is equivalent to CHEM 5302 at Carleton University.

Course Component: Lecture

CHM 8334 Novel Organic and Inorganic Molecules and Radicals (1.5 unit)

Topics to include neutralization-reionization techniques as well as flash pyrolysis and matrix isolation studies. This course is equivalent to CHEM 5009 at Carleton University.

Course Component: Lecture

CHM 8336 Non-Equilibrium Kinetics (1.5 unit)

Gas phase chemical kinetics of elementary and complex reaction mechanisms, as seen from a microscopic viewpoint. Unimolecular and bimolecular reactions under conditions of non-Boltzmann energy distributions. Consequences for combustion and atmospheric chemistry, as well as for fundamental kinetics. This course is equivalent to CHEM 5604 at Carleton University.

Course Component: Lecture

CHM 8337 Non-Linear Chemical Kinetics (1.5 unit)

Principles of non-linear dynamics as applied to very complex chemical reaction mechanisms containing feed-back processes. Monotonic, oscillatory, and chaotic dependence of concentrations on time. Gas phase and liquid phase reactions. This course is equivalent to CHEM 5605 at Carleton University.

Course Component: Lecture

CHM 8338 Unimolecular Reaction Dynamics: Experiment and Theory (1.5 unit)

Presentation of the theoretical models that have been developed for the understanding of unimolecular reactions, focussing on statistical theories such as RRKM theory. Experimental techniques for exploring the kinetics and mechanism of unimolecular reactions, including mass spectrometry, coincidence spectroscopy and ZEKE spectroscopy. This course is equivalent to CHEM 5100 at Carleton University.

Course Component: Lecture

CHM 8339 Heterogeneous Catalysis (1.5 unit)

Principles of catalytic reactions and topics in modern applications of catalysis. Bonding of substrates on surfaces; cluster-surface analogy; ensemble requirements; mechanisms of catalysis on metal and metal oxide surfaces. This course is equivalent to CHEM 5105 at Carleton University.

Course Component: Lecture

CHM 8340 Organotransition Metal Catalysis: E-H Bond Activation (1.5 unit)

Focus on the catalytic activation of E-H bonds by soluble organometallic complexes. Examples to include hydrogenation, hydrosilation and hydroboration catalysis, hydroamination and hydrophosphination. This course is equivalent to CHEM 5106 at Carleton University.

Course Component: Lecture

CHM 8341 Transition-Metal Catalyzed Polymerization (1.5 unit)

Recent developments in polymerization catalysis via transition metal complexes, including insertion, metathesis, and atom-transfer polymerization. Brief overview of relevant concepts in polymer chemistry (e.g. molecular weight, polydispersity, living polymerization, the glass transition). This course is equivalent to CHEM 5107 at Carleton University.

Course Component: Lecture

CHM 8343 Chemistry of the Main Group Elements (1.5 unit)

Fundamental and applied aspects of main group element chemistry. Topics may include non-metal chemistry, main group organometallic chemistry, application of main group element compounds to 3 uses of main group element compounds in synthesis. This course is equivalent to CHEM 5202 at Carleton University.

Course Component: Lecture

CHM 8344 Computational Approaches in Medicinal Chemistry (1.5 unit)

Theory and application of methods used in the pharmaceutical industry including molecular mechanics. This course is equivalent to CHEM 5602 at Carleton University.

Course Component: Lecture

CHM 8345 Molecular Energy Transfer (1.5 unit)

Principles of energy transfer during non-reactive molecular collisions as deduced from experiment and theory, mostly in the gas phase. Translational, rotational, vibrational and electronic energies are discussed. This course is equivalent to CHEM 5603 at Carleton University.

Course Component: Lecture

CHM 8346 Supercritical Fluids (1.5 unit)

Fundamental and practical aspects of the uses of supercritical fluids in the chemistry laboratory. Thermodynamic treatment of high pressure multicomponent phase equilibria, transport properties, solubilities, supercritical fluid extraction and chromatography for analytical purposes, reactions in supercritical fluids, equipment considerations, new developments. This course is equivalent to CHEM 5102 at Carleton University.

Course Component: Lecture

CHM 8348 Analytical Instrumentation (1.5 unit)

Principles of modern electronics, devices and instruments. Measurement of photonic and electrochemical signals. Conditioning of signals for feedback control and microcomputer interfacing. Computational data analysis techniques such as simplex optimization. Applications in chemical analysis include amperometric detector for capillary electrophoresis, and surface plasmon resonance immunosensor. This course is equivalent to CHEM 5500 at Carleton University.

Course Component: Lecture

CHM 8349 Free Radicals in Chemistry and Biology (1.5 unit)

Oxidative stress induced by free radicals plays a significant role in most fatal and chronic diseases. The chemistry of bio-radicals will be described and related to pathobiological processes such as lipid peroxidation and atherosclerosis, protein nitration and cross linking, and DNA scission. This course is equivalent to CHEM 5304 at Carleton University.

Course Component: Lecture

CHM 8352 Analytical Approach to Chemical Problems (1.5 unit)

Case study of analytical approach to various chemical problems in agricultural, biochemical, environmental, food processing, industrial, pharmaceutical and material sciences. Analytical methods include capillary electrophoresis, chemiluminescence, Fourier transform infrared spectroscopy, inductively coupled plasma emission spectroscopy, mass spectrometry, biochemical sensors, and fiber optics for remote sensing. This course is equivalent to CHEM 5501 at Carleton University.

Course Component: Lecture

CHM 8353 Trace and Ultratrace Analytical Chemistry (3 units)

Criteria for evaluation and selection of analytical techniques and methods. Electroanalytical techniques. Simultaneous and sequential multielement determination. Atomic absorption, atomic emission and atomic fluorescence spectrometry, using optical spectrometric and mass-spectrometric determination. Applications of these techniques at trace and ultratrace levels in complex matrices. This course is equivalent to CHEM 5502 at Carleton University.

Course Component: Lecture

CHM 8355 Trace Elemental Analysis Using Inductively Coupled Plasma Emission (Icp-Es) and Mass Spectrometry (I) (1.5 unit)

ICP-ES/MS techniques are among the most powerful tools presently available for elemental analysis for a wide range of interests such as environmental, geological and biological applications. The fundamentals, state of the art instrumentation, applications, existing challenges, and new research and developments will be covered.

Course Component: Lecture

CHM 8358 Advanced Topics in Biomolecular Sciences (1.5 unit)

Topics of current interest in biomolecular sciences and biological chemistry. Variable content from year to year. The course is equivalent to CHEM 5111 at Carleton University.

Course Component: Lecture

CHM 8359 Advanced Topics in Materials Chemistry (1.5 unit)

Topics of current interest in Materials Chemistry. Variable content from year to year. This course is equivalent to CHEM 5112 at Carleton University.

Course Component: Lecture

CHM 8360 Characterization Methods and Applications of Advanced Materials. (1.5 unit)

Detailed discussion of physico-chemical techniques from the practical and theoretical point of view. Topics covered will be chosen from the following: thermal analysis technics, optical spectroscopy, electrochemistry, X-ray and electron diffraction, electron microscopy, electron spectroscopies, magnetic resonance, and general instrumental methods. Applications related to materials science may include: field affect transistors, photovoltaics, light emitting devices, batteries, fuel cells, smart windows, and liquid crystalline displays. This course is equivalent to CHEM 5116 at Carleton University.

Course Component: Lecture

CHM 8361 Chemical Biology Part A (1.5 unit)

Overview of the field of Chemical Biology focussed on modern aspects of molecular science with applications to understanding biological mechanisms. Concepts such as biorthogonal chemistry, chemical genetics, expanded genetic codes and expanded genetic alphabets will be discussed in the context of how new chemical tools are developed and applied to understand and engineer living systems. Chemical probes for genomics, proteomics, metabolomics and vivo understanding of biology will be introduced with specific examples described. Genetically encoded probes will also be discussed. This course is equivalent to CHEM 5117 at Carleton University.

Course Component: Lecture

CHM 8362 Molecular Magnetism I (1.5 unit)

Metal containing paramagnetic molecules are omnipresent in chemistry and biochemistry. The presence of unpaired electron in a system has a drastic effect on physical properties of a molecule. Provides an introduction to the principles (Molecular Magnetism I) and advanced characterization of paramagnetic molecules (Molecular Magnetism II). Emphasis will be made on structure property relationship. This course will contain variable content from year to year by discussing recent progress on molecular magnetism. This course is equivalent to CHEM 5119 at Carleton University.

Course Component: Lecture

CHM 8363 Chemical Biology Part B (1.5 unit)

Overview of field of Chemical Biology focussed on modern aspects of molecular science with applications to understanding biological mechanisms. Concepts such as biorthogonal chemistry, chemical genetics, expanded genetic codes and expanded genetic alphabets will be discussed in the context of how new chemical tools are developed and applied to understand and engineer living systems. Chemical probes for genomics, proteomics, metabolomics and vivo understanding of biology will be introduced with specific examples described. Genetically encoded probes will also be discussed. This course is equivalent to CHEM 5118 at Carleton University.

Course Component: Lecture

CHM 8364 Molecular Magnetism II (1.5 unit)

Metal containing paramagnetic molecules are omnipresent in chemistry and biochemistry. The presence of unpaired electron in a system has a drastic effect on physical properties of a molecule. Provides an introduction to the principles (Molecular Magnetism I) and advanced characterization of paramagnetic molecules (Molecular Magnetism II). Emphasis will be made on structure property relationship. This course will contain variable content from year to year by discussing recent progress on molecular magnetism. This course is equivalent to CHEM 5121 at Carleton University.

Course Component: Lecture

CHM 8365 Communication in Chemistry (1.5 unit)

This course will involve a variety of activities over the semester, including an oral presentation. The three major modes of scientific communication will be covered: written, verbal, and visual communication. Students will be educated in best practices via lectures and assignments, and regular attendance at Departmental seminars. Graded work will include: a) writing a cover letter and CV, and abstract for a conference presentation. b) communicating research orally to scientific and non-scientific audiences, c) producing a scientific poster. Plagiarism will also be discussed. The course is focused on students producing the above deliverables, peer review of their work, and enhancing student capacity to engage and communicate beyond a specialist academic audience.

Course Component: Lecture

CHM 8714 Électrochimie interfaciale (1.5 crédit)

Introduction aux processus électrochimiques. Double couche électrique. Transfert de charge. Théorie du transfert d'électrons, cinétique électrochimie et électrocatalyse.

Volet : Cours magistral

CHM 8722 Sujets choisis de la chimie de coordination (1.5 crédit)

Introduction des concepts fondamentaux de la chimie de coordination. Discussions des sujets suivants : fixation du dioxyde de carbone et de l'azote, activation, méthanèse d'oléfines, liaison métal-métal.

Volet : Cours magistral

CHM 8723 Méthodes de la mécanique quantique - théorie (1.5 crédit)

Description de la théorie sur laquelle sont basées les méthodes de chimie quantique (HF, MPS, CI, DFT).

Volet : Cours magistral

CHM 8958 Projet de recherche / Research Proposal

Préparation d'un projet de recherche, sans rapport avec le sujet de thèse, à soutenir oralement devant un comité d'examen. L'étudiant doit démontrer sa capacité à défendre et justifier le mérite scientifique, la méthodologie, l'importance et la nouveauté du projet. Il doit réussir ce cours dans l'année qui suit la réussite de l'examen général. Les étudiants dont les résultats ne seraient pas satisfaisants peuvent se réinscrire une fois et doivent alors réussir en une session. / Preparation of a research project, unrelated to the thesis topic, to be defended orally before an examining committee. Student required to demonstrate the ability to defend and justify the scientific merit, methodology, importance, and novelty of the project. Must be completed within one year of passing the comprehensive examination. Students who fail this activity may re-register for it once and must then successfully complete it within one session.

Volet / Course Component: Recherche / Research

CHM 9998 Examen général de doctorat / Ph.D. Comprehensive

Volet / Course Component: Recherche / Research

TOX 5129 Adverse Outcome Pathways: A Framework to Support the Modernization of Chemical Risk Assessment (3 units)

This course will introduce the Adverse Outcome Pathway (AOP) framework and how it can be used to support the integration of modern test methods (e.g. in silico, in vitro, high throughput, etc..) into the chemical risk assessment process. Students will first learn about current practices and recent advances in both human health and ecological chemical risk assessment. Then students will receive an advanced introduction to the AOP framework, including the theory of AOPs, how they can be used in regulatory toxicology for facilitating the use of mechanistic data, test paradigm development, and risk assessment, and training on best practices for contributing to the AOP knowledge base. This will include in-class case studies on AOP development and a final assignment where student will be responsible for developing a novel AOP for a specific toxicity.

Course Component: Lecture

TOX 8156 Principles of Toxicology (3 units)

The basic theorems of toxicology with examples of current research problems. The concepts of exposure, hazard and risk assessment will be defined and illustrated with experimental material from some of the more dynamic areas of modern research. This course is equivalent to BIOL 6402 at Carleton University.

Course Component: Lecture

TOX 8158 Environmental Chemistry and Toxicology (3 units)

Overview of environmental chemistry and toxicology principles including chemical sources, fate, and effects in the environment. Examining organic reactions occurring in abiotic environments and biological systems, study aspects of toxicant disposition and biotransformation. Emphasis on contemporary problems in human health and the environment.

Course Component: Lecture

TOX 9104 Ecotoxicology (3 units)

Selected topics and advances in ecotoxicology with emphasis on the biological effects of contaminants. The potential for biotic perturbation resulting from chronic and acute exposure of ecosystems to selected toxicants will be covered along with the methods pesticide, herbicide and pollutant residue analysis and the concept of bound residues. This course is equivalent to BIOL 6403 at Carleton University.

Course Component: Lecture

TOX 9105 Seminar in Toxicology (3 units)

A one-session course in seminar format highlighting current topics in toxicology. The student will present a seminar and submit a report on the seminar topic. Student, faculty and invited seminar speakers.

Course Component: Seminar

TOX 9106 Genetic Toxicology (3 units)

Topics in mutagenesis and DNA repair, including spontaneous and induced mutagenesis, genetic toxicology testing, the genetics and biochemistry of replication, DNA repair and recombination, and the role of mutagens in the development of genetic disease and cancer. This course is equivalent to BIOL 6406 at Carleton University.

Course Component: Lecture

TOX 9107 Toxicology and Regulation (3 units)

This course will help students develop the understanding and skills to apply research results in toxicology to real-world needs for the management of risks posed by environmental contaminants as well as the development of regulation and policy involving such management.

Course Component: Lecture