

OFFICIAL UNDERGRADUATE COURSE OUTLINE FORM

Note: The University reserves the right to amend course outlines as needed without notice.

Course Code and Number: CHEM 422		Number of Credits: 4 Course credit policy (105)																	
Course Full Title: Principles and Methods of Molecular Modeling, Course Short Title (if title exceeds 30 characters): Molecular Modeling																			
Faculty: Faculty of Science		Department (or program if no department): Chemistry																	
Calendar Description: An introduction to modern computational techniques used for modeling physico-chemical properties of molecular and biomolecular systems, including empirical force field and quantum mechanical descriptions of individual molecules, as well as simulations of aggregate systems using molecular dynamics and Monte Carlo. The lecture course is accompanied by a computer lab where students will obtain practical experience in applying these techniques.																			
Prerequisites (or NONE):		CHEM 213, MATH 111, MATH 112, and one of the following: (PHYS 105 or PHYS 111). Note: As of January 2017, prerequisites will change to the following: CHEM 113, CHEM 114, MATH 111, PHYS 111, one of (MATH 112 or MATH 118), one of (PHYS 105 or PHYS 112), and one of the following: ([CHEM 213 and CHEM 224] or [instructor's permission for upper-level science students]). Note: CHEM 224 and MATH 211 are recommended.																	
Corequisites (if applicable, or NONE):																			
Pre/corequisites (if applicable, or NONE):																			
Equivalent Courses (cannot be taken for additional credit) Former course code/number: Cross-listed with: Equivalent course(s): <i>Note: Equivalent course(s) should be included in the calendar description by way of a note that students with credit for the equivalent course(s) cannot take this course for further credit.</i>		Transfer Credit Transfer credit already exists: <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No Transfer credit requested (OReg to submit to BCCAT): <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No (if yes, fill in transfer credit form) Resubmit revised outline for articulation: <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No To find out how this course transfers, see bctransferguide.ca .																	
Total Hours: 78 Typical structure of instructional hours:		Special Topics Will the course be offered with different topics? <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No If yes, different lettered courses may be taken for credit: <input type="checkbox"/> No <input type="checkbox"/> Yes, repeat(s) <input type="checkbox"/> Yes, no limit <i>Note: The specific topic will be recorded when offered.</i>																	
<table border="1"> <tr><td>Lecture hours</td><td>45</td></tr> <tr><td>Seminars/tutorials/workshops</td><td></td></tr> <tr><td>Laboratory hours</td><td>33</td></tr> <tr><td>Field experience hours</td><td></td></tr> <tr><td>Experiential (practicum, internship, etc.)</td><td></td></tr> <tr><td>Online learning activities</td><td></td></tr> <tr><td>Other contact hours:</td><td></td></tr> <tr><td>Total</td><td>78</td></tr> </table>		Lecture hours	45	Seminars/tutorials/workshops		Laboratory hours	33	Field experience hours		Experiential (practicum, internship, etc.)		Online learning activities		Other contact hours:		Total	78	Maximum enrolment (for information only): 24 Expected frequency of course offerings (every semester, annually, every other year, etc.): every other year	
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Department / Program Head or Director: David Fenske		Date approved: Sept. 28, 2015																	
Faculty Council approval		Date approved: November 6, 2015																	
Campus-Wide Consultation (CWC)		Date of posting: February 12, 2016																	
Dean/Associate VP: Lucy Lee		Date approved: November 6, 2015																	
Undergraduate Education Committee (UEC) approval		Date of meeting: February 26, 2016																	

Learning Outcomes

Upon successful completion of this course, students will be able to:

- describe the advantages and limitation of each of the molecular modeling techniques;
- critically select and apply the appropriate technique to modeling of a chemical or biochemical system;
- perform computer simulations using standard molecular modeling techniques;
- interpret the results of these simulations.

Prior Learning Assessment and Recognition (PLAR)

Yes No, PLAR cannot be awarded for this course because

Typical Instructional Methods (guest lecturers, presentations, online instruction, field trips, etc.; may vary at department's discretion)

Lectures, Computer Labs, Problem Solving

Grading system: Letter Grades: Credit/No Credit: Labs to be scheduled independent of lecture hours: Yes No

NOTE: The following sections may vary by instructor. Please see course syllabus available from the instructor.

Typical Text(s) and Resource Materials (if more space is required, download Supplemental Texts and Resource Materials form)

Author (surname, initials)	Title (article, book, journal, etc.)	Current ed.	Publisher	Year
1. Leach, A.	Molecular Modeling	<input checked="" type="checkbox"/>	Pearson	2001
2.		<input type="checkbox"/>		
3.		<input type="checkbox"/>		
4.		<input type="checkbox"/>		
5.		<input type="checkbox"/>		

Required Additional Supplies and Materials (software, hardware, tools, specialized clothing, etc.)**Typical Evaluation Methods and Weighting**

Final exam:	40%	Assignments:	Midterm exam: (2)	30%	Practicum:	%
Quizzes/tests:	%	Lab work:	Field experience:	%	Shop work:	%
Other:		Other: Computer Labs	30%	Other:	Total:	100%

Details (if necessary):**Typical Course Content and Topics**

Molecular geometry.
 Conformational analysis of simple systems
 Empirical force fields
 Quantum mechanical methods.
 Potential energy surface and energy minimization.
 Conformations of large molecules
 Molecular dynamics and Monte Carlo techniques
 Introduction to computer-aided drug design

Computer Lab Topics

Introduction to GaussView and Gaussian software.
 Energy optimization and frequency calculations.
 Cartesian, internal, and redundant coordinates.
 Stretch, bend, and torsion energy profiles.
 Potential energy surfaces.
 Reaction coordinate and reaction profiles.
 Calculation of classical reaction rates using Eyring equation
 Tunneling corrections to classical reaction rates
 Isotope effects
 Transition state optimization techniques