UNIVERSITY OF THE FRASER VALLEY

ORIGINAL COURSE IMPLEMENTATION DATE: September 2001
REVISED COURSE IMPLEMENTATION DATE: January 2017
COURSE TO BE REVIEWED: (six years after UEC approval) February 2022
Course outline form version: 09/15/14

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 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):

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.

Transfer Credit

Transfer credit already exists: ☐ Yes ☒ No

Transfer credit requested (OReg to submit to BCCAT):
☐ Yes ☒ No (if yes, fill in transfer credit form)

Resubmit revised outline for articulation: ☐ Yes ☒ No

To find out how this course transfers, see **bctransferguide.ca**.

Total Hours: 78

Typical structure of instructional hours:

Lecture hours	45
Seminars/tutorials/workshops	
Laboratory hours	33
Field experience hours	
Experiential (practicum, internship, etc.)	
Online learning activities	
Other contact hours:	
Total	**78**

Special Topics

Will the course be offered with different topics?
☐ Yes ☒ No

If yes, different lettered courses may be taken for credit:
☐ No ☐ Yes, repeat(s) ☐ Yes, no limit

Note: The specific topic will be recorded when offered.

Maximum enrolment (for information only): 24

Expected frequency of course offerings (every semester, annually, every other year, etc.): every other year

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	☒	Pearson	2001
2.			☐		
3.			☐		
4.			☐		
5.			☐		

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