

**UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE OUTLINE
FALL 2017**

1. Course: CHEMISTRY 599.11 / 689.07 – Modeling Multiscale Systems

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	EMAIL	OFFICE HOURS
L01/L02	TR	12:30-13:45	SA 107	Dennis Salahub	BI 556	dsalahub@ucalgary.ca	By email appt.

Desire 2 Learn course name [CHEM 599 L02 - \(Fall 2017\) - Selected Topics in Chemistry](#)

Desire 2 Learn course name [CHEM 689 L01 - \(Fall 2017\) - Selected Topics in Physical Chemistry](#)

Departmental Office: Room SA 229, Tel: (403) 220-5341, e-mail: chem.undergrad@ucalgary.ca

To avoid IT problems, it is recommended that the students use their U of C account for all course correspondence.

- 2. Prerequisites:** Chemistry 371, Chemistry 373 or equivalent or consent of instructor
<http://www.ucalgary.ca/pubs/calendar/current/chemistry.html#6525>
- 3. Grading:** The University policy on grading and related matters is described sections [F.1](#) and [F.2](#) of the online University Calendar. In determining the overall grade in the course the following weights will be used:

Undergraduates (599.11)		Graduates (689.07)	
Midterm report and oral	30%	Critical review on special topics and oral	30%
Hands-on projects	40%	Hands-on projects and mentoring	40%
Final report and oral	30%	Final research proposal and oral	30%

Total	100%		100%

The marks for each of the course components will be recorded as numerical scores and combined to arrive at a final numerical score, which will be converted to the letter grade that is reported to the Registrar.

Approximate Grading Scale:

A+	A	A-	B+	B	B-
95% - 100%	86% - 94%	82% - 85%	77% - 81%	74% - 76%	71% - 73%
C+	C	C-	D+	D	F
67% - 70%	61% - 66%	57% - 60%	54% - 56%	50% - 53%	< 50%

- 4. Missed Components of Term Work:** The regulations of the Faculty of Science pertaining to this matter are found in the Faculty of Science area of the Calendar in [Section 3.6](#). It is the student's responsibility to familiarize himself/herself with these regulations. See also [Section E.6](#) of the University Calendar.

There are no deferred Midterm/ term test examinations. In the event that a student misses the midterm or any course work due to illness then an official medical note will be required. Absences must be reported **within 48 hrs**. If a student misses the midterm for other reasons, then analogous documentation will be required. The course coordinator will need to see the original documentation (not electronic copy) for review / decision and keep it (or a copy) for their records. The documentation must be provided to the course coordinator **within 15 days** of the date of the midterm in order for an excused absence to be considered. If an excused absence is approved, then the percentage weight of a legitimately missed midterm examination *will be pro-rated among the remaining components of the course* (see [Section E.3](#) of the University Calendar)].

- 5. Examination Policy:** Reports and projects are “take home”. All materials may be referenced. Course materials may be brought for reference at oral examinations. Students should also read the Calendar, [Section G](#), on Examinations.

6. Course Materials: Suggested references (plus material will be posted on D2L)

1. Szabo and Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Macmillan, NY.
2. Parr and Yang, Density Functional Theory of Atoms and Molecules, Oxford University Press, NY
3. Heine, Joswig and Gelessus, Computational Chemistry Workbook, Wiley-VCH, Weinheim
4. deMon Users' Guide, <http://demon-software.com>
5. NAMD and VMD Users' Guides and Tutorials, <http://www.ks.uiuc.edu/Research/namd/>
6. Leach, Molecular Modeling, Principles and applications, Prentice Hall, Harlow
7. Frenkel and Smit, Molecular Simulation, from algorithms to applications, Academic, London

7. Writing across the curriculum statement: For all components of the course, in any written work, the quality of the student's writing (language, spelling, grammar, presentation etc.) will be a factor in the evaluation of those reports. See also [Section E.2](#) of the University Calendar.

8. Reappraisal of Grades: Students should be aware that the grade being reappraised may be raised, lowered or remain the same. See [Section I.3](#) of the University Calendar.

(a) **Term work:** A student who feels that a piece of graded term work (term paper, essay, test, etc.) has been unfairly graded, may have the work re-graded. The student shall discuss the work with the Instructor **within 15 days** of either being notified about the mark, or of the item's return to the class. If not satisfied, the student shall immediately submit the *Reappraisal of Term work Grade* form to the Associate Head of Chemistry, Dr. Farideh Jalilehvand (ahugchem@ucalgary.ca), who will arrange for a reassessment of the work if, and only if, the student's argument is valid. *Note:* Students should attempt to present their rational as effectively and as fully as possible. Mere dissatisfaction with a decision is not sufficient grounds for the appeal of a grade, or other academic decision. See sections [I.1](#) and [I.2](#) of the University Calendar.

(b) **Final Exam:** A student wishing a reappraisal of the final grade should first attempt to review the final assessment with the department offering the course. If not satisfied, the student shall submit the request to the Enrolment Services. See [Section I.3](#) of the University Calendar.

9. OTHER IMPORTANT INFORMATION FOR STUDENTS:

(a) **Misconduct:** Academic misconduct (cheating, plagiarism, or any other form) is a very serious offence that will be dealt with rigorously in all cases. A single offence may lead to disciplinary probation or suspension or expulsion. The Faculty of Science follows a zero tolerance policy regarding dishonesty. Please read the sections of the University Calendar under [Section K](#) on Student Misconduct to inform yourself of definitions, processes and penalties. Examples of academic misconduct include but are not limited to: submitting or presenting work as if it were the student's own work when it is not; submitting or presenting work in one course which has also been submitted in another course without the instructor's knowledge; borrowing experimental values from others without the instructor's approval; falsification/ fabrication of experimental values in a lab report; copying materials from written or electronic resources; non-authorized recording of lectures.

(b) **Assembly Points:** In case of emergency during class time, be sure to FAMILIARIZE YOURSELF with the information on [assembly points](#).

(c) **Academic Accommodation Policy:** Students needing an Accommodation because of a Disability or medical condition should contact Student Accessibility Services in accordance with the Procedure for Accommodations for Students with Disabilities available at http://www.ucalgary.ca/policies/files/policies/procedure-for-accommodations-for-students-with-disabilities_0.pdf. Students needing an Accommodation in relation to their coursework or to fulfill requirements for a graduate degree, based on a Protected Ground other than Disability, should communicate this need, preferably in writing, to their Instructor/ Course Coordinator. Religious accommodation requests relating to class, test or exam scheduling or absences must be submitted no later than **14 days** prior to the date in question: <http://www.ucalgary.ca/pubs/calendar/current/e-4.html>

(d) **Safewalk:** Campus Security will escort individuals day or night (<http://www.ucalgary.ca/security/safewalk/>). Call (403) 220-5333 for assistance. Use any campus phone, emergency phone or the yellow phones located at most parking lot pay booths.

(e) **Freedom of Information and Privacy:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPP). As one consequence, students should identify themselves on all written work by placing their name on the front page and their ID number on each subsequent page. For more information see also <http://www.ucalgary.ca/secretariat/privacy>.

- (f) **Student Union Information:** VP Academic Phone: (403) 220-3911 email: suvpaca@ucalgary.ca
SU Faculty Rep. Phone: (403) 220-3913 e-mail: science1@su.ucalgary.ca, science2@su.ucalgary.ca and
science3@su.ucalgary.ca; Student Ombuds Office: (403) 220-6420 e-mail ombuds@ucalgary.ca
<http://ucalgary.ca/provost/students/ombuds>
- (g) **Internet and Electronic Device Information:** You can assume that in all classes that you attend, your cell phone should be turned off unless instructed otherwise. Also, communication with other individuals, via laptop computers, Blackberries or other devices connectable to the Internet is not allowed in class time unless specifically permitted by the instructor. If you violate this policy you may be asked to leave the classroom. Repeated abuse may result in a charge of misconduct.
- (h) **U.S.R.I.:** At the University of Calgary, feedback provided by students through the Universal Student Ratings of Instruction (USRI) survey provides valuable information to help with evaluating instruction, enhancing learning and teaching, and selecting courses (www.ucalgary.ca/usri). Your responses make a difference - please participate in USRI Surveys.

Department Approval: Approved by Department Head

Date: August 23, 2017

Associate Dean's Approval for

Alternate final examination arrangements: Approved by Associate Dean

Date: August 23, 2017