UNIVERSITY OF CALGARY

DEPARTMENT OF CHEMISTRY
COURSE OUTLINE
FALL 2014

1. Course: CHEMISTRY 689.07 – Modeling Multiscale Systems
Lecture Sections:

L01: two 75-minute lectures, time and place to be determined in consultation with the students. Instructor, Dennis Salahub Office BI556 Tel. No., 220 3720 e-mail address, dennis.salahub@ucalgary.ca Office Hours: Monday 13:00 – 16:00

Desire 2 Learn (D2L) course name, CHEM 689 – Multiscale Modeling

2. Prerequisites: Chemistry 371, Chemistry 373 or equivalent or consent of the Instructor. (**http://www.ucalgary.ca/pubs/calendar/current/chemistry.html#6525**).

Note: The calendar description and the Faculty of Science policy on prerequisites and antirequisites is described in section 3.5 C. of the online University Calendar (**http://www.ucalgary.ca/pubs/calendar/current/sc-3-5.html**). Students are responsible to ensure that they meet all prerequisite requirements for each course in which they are registered. Students who do not meet these requirements will be deleted from the course.

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:

Critical review on special topics and oral	30%
Hands-on projects	40%
Final research proposal and oral	30%
Total	100%

The marks for each of the course components will be recorded as a numerical score and combined as shown above to arrive at the total numerical score which will then be converted to a letter grade to be 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

5. 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

6. Examination Policy: All examinations will be either of the form of reports to be submitted prior to an oral examination or reports of hands-on modelling projects.

Students should also read the Calendar, Section G, on Examinations.

7. Approved Mandatory and Optional Course Supplemental Fees: The Department of Chemistry has a laboratory glassware breakage fee. At the start of the course, each student is assigned a locker and checks-in to establish that they have a complete set of usable glassware. By signing for check-in, a student agrees that they are now responsible for the glassware until check out. Any equipment that is missing, unusable or has been replaced during the semester will be charged to the student. All students, even those who withdraw early from the course must check out of the laboratory before the last day of lectures. Any student who fails to check out before the last day of lectures for the term will be assessed a charge of $30.00. If this fee is not paid by the last day of the final examination period of the term, an additional $10.00 administrative fee will be charged and university services (registration, transcripts, etc.) may be withheld.

8. Writing across the curriculum statement: In this course, the quality of the student's writing in laboratory reports will a factor in the evaluation of those reports. See also Section E.2 of the University Calendar.

9. OTHER IMPORTANT INFORMATION FOR STUDENTS:

(a) 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. Student Misconduct to inform yourself of definitions, processes and penalties

(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 with documentable disabilities are referred to the following links: Calendar entry on students with disabilities and Student Accessibility Services.

(d) Safewalk: Campus Security will escort individuals day or night (http://www.ucalgary.ca/security/safewalk/). Call 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: 220-3911 Email: suvpaca@ucagary.ca.
SU Faculty Rep. Phone: 220-3913 Email: sciencerep@su.ucalgary.ca; Student Ombudsman

(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) 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 18 2014