

UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
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.

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

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

2. TEXTBOOKS: 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

TOPICS COVERED AND SUGGESTED READING:

1. Multiscale modeling – what and why?
2. Quantum chemistry, electronic structure theory
 - a. Many-electron wave functions and the Hartree-Fock method
 - b. Density Functional Theory
 - i. Hohenberg-Kohn theorem
 - ii. Kohn-Sham Equations
 - iii. Implementation with Gaussian orbitals - deMon
3. Molecular Dynamics
 - a. Newtonian mechanics
 - b. Empirical force fields
 - c. Simulation algorithms - CHARMM
 - d. Applications using NAMD for small models – ion solvation
 - e. Applications to proteins or other complex simulations

LABORATORY EXPERIMENTS:

Hands-on exercises and projects using deMon and NAMD software

Department Approval: Approved by Department Head

Date: August 23, 2017