UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
FALL 2016

COURSE: CHEMISTRY 689.07, Modeling Multiscale systems

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	PHONE	EMAIL	OFFICE HOURS
L01	TuTh	2:00-3:15	ST 063	Dr. Dennis Salahub	BI 556	220-3720	dsalahub@ucalgary.ca	By email appt.

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 17 2016