UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
FALL 2016

COURSE: CHEMISTRY 575, Advanced Electronic Structure Theory

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	PHONE	EMAIL	OFFICE HOURS
L01	MWF	8:00-8:50	SA 017	Dr. Dennis Salahub	BI 556	220-3720	dsalahub@ucalgary.ca	By appt.
T01	TU	8:00-8:50	SA 017	Dr. Dennis Salahub				
B01	M	13:00-16:00	SA 204	TA (TBD)				

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. Cramer, Essentials of Computational Chemistry: Theories and Models, Wiley, Chichester.
3. Jensen, Introduction to Computational Chemistry, Wiley, Chichester.
4. Helgaker, Jorgensen and Olsen, Molecular Electronic-Structure Theory, Wiley, Chichester.
5. Parr and Yang, Density Functional Theory of Atoms and Molecules, Oxford University Press,NY
6. Koch and Holthausen, A Chemist's Guide to Density Functional Theory.
7. Heine, Joswig and Gelessus, Computational Chemistry Workbook, Wiley-VCH, Weinheim
8. deMon Users' Guide, http://demon-software.com

TOPICS COVERED IN LECTURES (To be finalized in consultation with the students)

Monday, Sept. 12	**Motivation, why study electronic structure theory, multiscale modeling of complex systems**
Wednesday, Sept 14	**Symmetry of a many-electron wave function - I**
Friday, Sept 16	**Symmetry of a many-electron wave function - II**
Monday, Sept 19	**Electron Spin**
Wednesday, Sept 21	**Many-electron Hamiltonian of a molecular system**
Friday, Sept 23	**Slater rules for the calculation of matrix elements involving determinants - I**
Monday, Sept 26	**Slater rules for the calculation of matrix elements involving determinants - II**
Wednesday, Sept 28	**Variational theory - I**
Friday, Sept 30	**Variational theory - II**
Monday, Oct 3	**Variational perturbation theory - I**
Wednesday, Oct 5	**Variational perturbation theory - I**
Friday, Oct 7	**Self-consistent field theory**
Wednesday, Oct 12	**Hartree-Fock SCF theory - I**
Friday, Oct 14	**Hartree-Fock SCF theory - II**
Monday, Oct 17	**The Roothan equations: LCAO-MO-HF-SCF**
Wednesday, Oct 19	**Density matrices**

Department Approval: Approved by Department Date: August 17 2016

Friday, Oct 21	**Density Functional Theory – an overview**
Monday, Oct 24	**Hole functions**
Wednesday, Oct 26	**Hole functions/local spin density approximation**
Friday, Oct 28	**General DFT**
Monday Oct 31	**Geometry optimization**
Wednesday, Nov 2	**Vibrational frequencies and normal modes**
Friday, Nov 4	**Transition states and reaction paths**
Monday Nov 7	**External electric field**
Wednesday, Nov 9	**External magnetic field**
Monday, Nov 14	**Ground-state Hessian**
Wednesday, Nov 16	**Coupled perturbed Kohn-Sham theory - I**
Friday, Nov 18	**Polarization**
Monday, Nov 21	**Coupled perturbed Kohn-Sham theory - II**
Wednesday, Nov 23	**Magnetization**
Friday, Nov 25	**NMR spin coupling**
Monday, Nov 28	**Excitation energies**
Wednesday, Nov 30	**Combined quantum mechanics/molecular mechanics (QM/MM)**
Friday, Dec 2	**Student project presentations – Session 1**
Monday, Dec 5	**Student project presentations – Session 2**
Wednesday, Dec 7	**Student project presentations – Session 3**
Friday, Dec 9	**Student project presentations – Session 4**

TOPICS COVERED IN TUTORIALS (To be finalized in consultation with the students)

Tutorial drills will be assigned, at the latest, by Monday noon, starting with the second week of lectures. Written answers must be submitted by the following Monday noon. The written answers will be assigned a tentative grade by the Instructor. In the following tutorial session on Tuesday morning students will be invited to present their work (using a document projector) and, with some guidance from the Instructor, to correct mistakes. A final grade will then be assigned by the Instructor.

Tutorial schedule:

September 20	**Planning session to make sure everyone is clear on the rules of engagement and to identify any issues arising from the first 4 lectures and the first lab**
September 27	**Many-electron wave functions and determinants**
October 4	**Matrix elements involving many-electron wave functions**
October 11	**Matrix elements involving many-electron wave functions using the Slater rules**
October 18	**Matrices and eigenfunctions**
October 25	**Perturbation theory**
November 1	**Hartree-Fock equations**
November 8	**Density matrices**
November 15	**DFT and energy gradient**
November 22	**Energy gradient**
November 29	**Perturbed Kohn-Sham - I**
December 6	**Perturbed Kohn-Sham - II**

TOPICS COVERED IN LABORATORIES (To be finalized in consultation with the students)

LABORATORY INTRODUCTION: A document will be posted on D2L explaining how the computational lab will work
LABORATORY EXPERIMENTS: Detailed instructions for each of the labs will be posted on D2L

Lab schedule:

September 19	**Getting started, the GUI (Gabedit), DFT engine (deMon2k) and the analyzer (Molden)**
September 26	**Molecules and molecular orbitals**
October 3	**Details of a calculation**
October 17	**Geometry optimization**
October 24	**Chemical reactions**
October 31	**The second derivative of the energy**
November 7	**Electronic spectroscopy**
November 14	**NMR and EPR spectra**
November 21	**QM/MM for solvation**
November 28	**Project**