SYLLABUS

Time:	Mon./Wed./Fri. 9:40-10:30 am
Location:	PS H230
Instructor:	Prof. Dmitry Matyushov Office: PS D202E Phone: (480)9650057 E-mail: dmitrym@asu.edu Office hours: Mondays and Wednesdays, 10:30 - 11:30 am
Text:	Modern Quantum Chemistry. Introduction to Advanced Electronic Structure Theory, by Attila Szabo and Neil S. Ostlung
Web page:	`http://www.public.asu.edu/ dmatyus/ teaching/chm546/chm546.html`
Optional Texts:	Introduction to Computational Chemistry, by F. Jensen (Wiley, New York, 1999) Density-Functional Theory of Atoms and Molecules, by R. G. Parr and W. Yang (Oxford University Press, 1989)

GRADING:

Homework: Five homework assignments will be given during the semester. Each of them must be turned in by 6:00 PM on the due date. The homework assignments will make 50 % of the grade. In addition, assignments to perform simple *ab initio* calculations to test your understanding of the material will be assigned periodically. These are not graded, but should be completed by the given deadline. The solution for the problems should be stored in output files on the server and will be checked. Doing the problems is therefore necessary for satisfactory completion of the course.

Mid-term exam: A one-hour mid-term exam will be given in class (25 % of the grade, see schedule below).

Final exam: A cumulative, two-hour exam or a final project (to be decided), 25 % of the grade. All exams are open-book and open-notes.

ABSTRACT:
This course is designed to provide basic concepts and practical experience in electronic structure calculations. The goal is to cover enough theory to allow an "intelligent" use of modern electronic structure packages. In order to provide a hands-on experience in real calculations, a course account will be open on an Alpha/Linux workstation. The students will be able to perform calculations using the GAMESS package. The connection is through the Secure Shell (SSH) protocol. The OpenSSH software package is available free for various platforms. OpenSSH is installed on PCs in the Graduate Computer Lab (C3, access through the NMR lab).

TENTATIVE SCHEDULE OF CLASSES

Date	Topic
Jan. 14	Computer account and usage of GAMESS
Jan. 16	Wave functions and matrix representation of quantum mechanics
Jan. 18	Born-Oppenheimer approximation
Jan. 21 & 23	Linear algebra review (Chap. 1)
Jan. 25	The variation method
Jan. 28	Orbitals and Slater determinants
Jan. 30 & Mar. 1	Matrix elements
Mar. 4	The Hartree-Fock equation
Mar. 6	Koopmans' theorem and interpretation of HF solutions
Mar. 8	Midterm exam
Mar. 11	Restricted Closed-shell HF
Mar. 13	Roothaan equations
Mar. 15	Model calculations
Mar. 18	Polyatomic basis sets
Mar. 20	Closed-shell calculations
Mar. 22	Unrestricted open-shell HF
Mar. 25	Pople-Nesbet equations
Mar. 27–Apr. 1	Molecular symmetry groups
Apr. 3 – Apr. 12	CI calculations
Apr. 15 – Apr. 22	Density Functional Theory
Apr. 22 – 26	Perturbation Corrections

HOMEWORK ASSIGNMENTS AND EXAMS

Date due	Homework
Feb. 8	Homework 1
Feb. 25	Homework 2
Mar. 8	Midterm exam
Mar. 22	Homework 3
Apr. 5	Homework 4
Apr. 19	Homework 5
May 6	7:40–9:30, Final exam or project defense