Course Outline Chem 400 / Chem 740 :
Computational Quantum Chemistry

Instructor: Marcel Nooijen (Phys 2021, nooijen@uwaterloo.ca)

This course will provide a practical guide to quantum chemical calculations. The course will be held mainly in a computer lab setting, with students performing calculations under guidance of the instructor. In addition the lecture material will cover main topics in computational chemistry. A major component of the course is the computational research project. Each student in the class follows an individual trajectory, based on their interests and their choice of research project. The following topics will be covered:

- Electronic Structure Theory: Hartree-Fock, Density Functional Theory, MP2, CCSD(T), CASSCF, MRCI, MREOM, semi-empirical methods, basis sets, thermochemistry.
- Geometry optimizations: searching minima and transition states, vibrational frequencies, reaction path following.
- Calculations in solution. ONIOM calculations.
- Calculations of excited states.
- Multireference calculations for ground and excited states.
- Which method / basis set for what problem?
- Case studies: Gaining understanding from quantum chemical calculations.

We will use a small selection of electronic structure packages, with the aim to familiarize the students with different possibilities. Each student will select the topics that will be studied in detail, under the guidance of the instructor. The student will select topics of study , based on interest and the final project. The following programs will be used:

- Gaussian / Gaussview: Mostly used for ground state chemistry problems.
- ACES2: High accuracy quantum chemistry, excited states.
- MOLPRO: High accuracy quantum chemistry: potential energy surfaces
- ORCA: A fairly new electronic structure packages for larger molecules.
- ORCA & ACES2: Multireference treatment of transition metal complexes.
- GAMESS: High accuracy quantum chemistry.

A major part of the course is a computational research project that will be carried out in small groups of students (1-3), according to their research interests. Each group will present a report and an oral presentation of the project. For this project students will use computational chemistry packages suitable to their needs. Computer resources will be made available to carry out the research. It is important to start your project as early as possible. Computations take time, and if everybody is submitting 20 jobs near the end of class nothing gets done. Computer resources are finite!

The course essentially consists of a number of labs. I will broadly check that you worked your way through the excises, and ask you to tell me how much of the lab (~ biweekly) you got done (percentage wise). This will form the basis of the assignment part of the grade (40%). The final project, presentation and report will have a weight of 60%. There will not be a final exam.

Academic Integrity: In order to maintain a culture of academic integrity, members of the University of Waterloo community are expected to promote honesty, trust, fairness, respect and responsibility. [Check www.uwaterloo.ca/academicintegrity/ for more information.]

Appeals: A decision made or penalty imposed under Policy 70 (Student Petitions and Grievances) (other than a petition) or Policy 71 (Student Discipline) may be appealed if there is a ground. A student who believes he/she has a ground for an appeal should refer to Policy 72 (Student Appeals) www.adm.uwaterloo.ca/infosec/Policies/policy72.htm .

Discipline: A student is expected to know what constitutes academic integrity [check www.uwaterloo.ca/academicintegrity/ to avoid committing an academic offence, and to take responsibility for his/her actions. A student who is unsure whether an action constitutes an offence, or who needs help in learning how to avoid offences (e.g., plagiarism, cheating) or about "rules" for group work/collaboration should seek guidance from the course instructor, academic advisor, or the undergraduate Associate Dean. For information on categories of offences and types of penalties, students should refer to Policy 71, Student Discipline, www.adm.uwaterloo.ca/infosec/Policies/policy71.htm. For typical penalties check Guidelines for the Assessment of Penalties, www.adm.uwaterloo.ca/infosec/guidelines/penaltyguidelines.htm

Grievance: A student who believes that a decision affecting some aspect of his/her university life has been unfair or unreasonable may have grounds for initiating a grievance. Read Policy 70, Student Petitions and Grievances, Section 4, www.adm.uwaterloo.ca/infosec/Policies/policy70.htm. When in doubt please be certain to contact the department's administrative assistant who will provide further assistance.

Note for Students with Disabilities: The Office for persons with Disabilities (OPD), located in Needles Hall, Room 1132, collaborates with all academic departments to arrange appropriate accommodations for students with disabilities without compromising the academic integrity of the curriculum. If you require academic accommodations to lessen the impact of your disability, please register with the OPD at the beginning of each academic term.

Turnitin.com: Plagiarism detection software (Turnitin) will be used to screen assignments in this course. This is being done to verify that use of all material and sources in assignments is documented. In the first week of the term, details will be provided about the arrangements for the use of Turnitin in this course.

Note: students must be given a reasonable option if they do not want to have their assignment screened by Turnitin. See: http://uwaterloo.ca/academicintegrity/Turnitin/index.html for more information

A useful text book is:

Essentials of Computational Chemistry: Theories and models (second edition) by Christopher J. Cramer, Wiley, ISBN 0-470-09182-7
I will make sure some copies are in the library. There is no need to buy this book. I will be posting lecture notes.

Other reference reading material on computational quantum chemistry:

Introduction to Computational Chemistry by Frank Jensen, Wiley, ISBN 0-471 98425 6

Exploring Chemistry with Electronic Strucure Methods, J. B. Foresman and A Frisch, ISBN 0-9636769-3-8

Gaussian User's Reference, A Frisch, M. J. Frisch and G. W. Trucks, ISBN 0-9727187-0-2

References on Theoretical Background:

Quantum Chemistry by D. McQuarrie, University Science Books, ISBN 978-1-891389-50-4

Quantum Chemistry, fifth edition, Ira N. Levine, Prentice Hall, ISBN 0-13-685512-1

Modern Quantum Chemistry, Introduction to advanced Electronic Structure Theory, A. Szabo and N. S. Ostlund, McGraw-Hill, 1989, Dover edition, ISBN 0-486-69186-1