CHEM 3260: Introduction to Computational Chemistry
Course Syllabus

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Course Website: On UM Learn.

Place and Time: Lecture T/R 1:00-2:15pm, Tier 400

Lab: T 2:30-5:25pm, Machray Hall 108

Course Text and Other Literature

- Course text: E. G. Lewars, Computational Chemistry – *the (current) 3rd edition is available as pdf through the library*

Other literature:

- C. J. Cramer "Essentials of Computational Chemistry", 2nd ed., Wiley 2004
- Foresman, J. B.; Frisch, Æ. Exploring Chemistry with Electronic Structure Methods, 3rd ed.; Gaussian, Inc.: Wallingford, CT, 2015. (See also: http://expchem3.com/)
- Original or review literature as assigned from time to time
- *An excellent additional resource are the "Reviews in Computational Chemistry" published by Wiley and available through the library. See http://onlinelibrary.wiley.com/bookseries/10.1002/SERIES6143*

Reason for Course

The advent of computers that are ever faster and cheaper and the continual refinement of computational algorithms have led to the regular use of computational chemistry both in academic and industrial research. *For instance, a smartphone today has the same performance as the world's fastest supercomputer had in 1994!* Once the domain of computational chemistry experts, these advances have opened the door for experimental researchers to apply computational chemistry methods to solve problems and to make predictions. It has thus become increasingly important that all chemists be familiar with these methods and that they have some hands-on experience with computational chemistry software.

Course Objectives

The goals of the course are as follows:

(i) Students will develop **computational chemistry literacy**. This comprises the ability to understand general contents and critically evaluate quality and applicability of computational chemistry methods and results in the scientific literature.

(ii) Students will be able to perform **standard computational chemistry** tasks such as, for instance, geometry optimizations or free energy calculations including solvation.

Prerequisite Knowledge

Students are expected to have a basic understanding of quantum mechanical concepts such as the Schrödinger Equation, wave functions and molecular orbitals; in addition, students are expected to have a general chemist's understanding of basic molecular structure, reaction paths, thermodynamics, and an appreciation for problems in chemistry.

The formal course prerequisites for this course reflect these requirements:

- CHEM2260 (or its predecessor CHEM2280) provides students with an introduction to quantum-chemical concepts.
- The formal requirement, six credit hours out of CHEM2210, CHEM2220, CHEM 2290, CHEM2370, CHEM2400, CHEM3400 ensures that students have sufficient knowledge of basic chemical concepts: "If you wish to model chemistry, you need to first know the chemistry to model."
- It is *recommended* that students have taken CHEM2290: This course provides an introduction to thermodynamics – which underlies many of the approaches and concepts taught in the current course.

Description and Scope

The field of computational chemistry encompasses the development and application of numerical methods for the study of chemical systems. The successful investigation of problems in chemistry using computational chemistry requires both an understanding of the nature of the chemistry being studied and an understanding of the computational methods employed. The theoretical framework of computational chemistry methods will be presented briefly, as far as necessary for understanding the methods. Emphasis will be placed on practical understanding of the strengths, weaknesses, and ranges of applicability of different methods. This knowledge will allow for the critical evaluation of the validity and accuracy of results and of the conclusions derived from the computational chemistry modelling of particular chemical problems. The laboratory component provides an introduction to the use of computational chemistry software. The following topics will be discussed:

- Empirical force field models and their use in chemical and biochemical studies.
- Potential energy surfaces and the exploration tools available for the location of local and global minima and transition states.
- Electronic structure models for the prediction of energies, thermodynamic quantities, geometries, and electronic and spectral properties.
- The solvation process and the incorporation of its effects in molecular modelling.
- Considerations, strategies, and goals in setting up computational chemistry studies.

Course Format
The course will have lecture (3 lecture hours, 150min, per week) and laboratory (3 hours per week) components.

Detailed course outline

The following list is a tentative outline, still subject to adjustment. Accordingly, the exact content and order given may change.

	Subject
1	Introduction: The subject of computational chemistry and its tools
2	Potential energy surface (PES); geometry optimization
3	Empirical force fields, molecular mechanics (MM)
4	Thermodynamics *(brief review)*
5	Basic concepts from quantum mechanics
6	Ab initio: MO theory; SCF theory
7	Hartree-Fock method *and related technical issues* - Basis sets - Basis set superposition error (BSSE) - Effective core potentials (ECP) *etc.*
8	Post-Hartree-Fock methods - Electron correlation
9	Semiempirical methods
10	Density functional theory (DFT)
11	Property calculation - Excited states (including time-dependent DFT, TD-DFT) - Spectroscopic observables
12	Solvation models - Atomic charges
13	Analysis tools - AIM (Bader) analysis, NBO *etc.*
14	Extra topics – *time permitting* - Parallel computing - Heavy elements and relativity - Dynamics - Machine learning *etc.*

Course evaluation

Assignments	8%
Midterm examination	23%
Final examination	44%
Laboratory	25%

Note: There is a separate passing criterion for the lab (50%) component of the course, i.e. a lab mark below 50% will result in an overall course grade of F.

Grading scheme: The conversion to final letter grades will be as follows: A+ (87% – 100%), A (81–86%), B+ (75–80%), B (69–74%), C+ (63 – 68%), C (56–62%), D (50–55%) F (< 50%)

Exams

Both exams (midterm and final) will be take-home exams. The exact timing will be determined in consultation between instructor and students, so as to reduce conflict with other exams as much as possible.

Final examination and grades policies can be found at: http://umanitoba.ca/admin/governance/governing_documents/academic/1299.html

Assignments

Assignments will cover theoretical aspects of the course. I am planning to distribute 5 assignments. The assignments will normally be due one week after being made published, with the marks being available within one week of the due date.
Dates for release of assignments: Jan. 16, Jan. 30, Feb. 13, Mar. 12, Mar. 26
Changes to this schedule (if any) will be determined in consultation with the class.

Laboratory

The field of computational chemistry encompasses development and application of numerical methods for the study of chemical systems. The successful investigation of problems in computational chemistry requires not only an understanding of the general theory, applicability and limitations of the methods (which are discussed in the lecture) but also practical, hands-on experience of setting up, running and trouble-shooting actual calculations. This is the subject of the laboratory. *Laboratory attendance is mandatory*.
In the laboratory, students will

- Gain working knowledge of the LINUX operating system, including basic commands, editors and so on;
- Gain experience in the use of the Gaussian software and its Graphical User Interface (GUI);
- Set up, run, monitor and trouble-shoot simple calculations (e.g. geometry optimizations, property calculations);
- Extract useful information from their calculations (e.g. energetics, molecular orbitals);
- Compare different methods and levels of theory, so as to gain practical experience of their respective cost and accuracy.

Laboratory Schedule (Tentative)

The following computational experiments will be performed.

(1) Introduction to Gaussian 16 (G16) and to GaussView (GaussView is the graphical user interface, GUI)
  - GUI usage
  - Input files (Z-matrix)
  - Output files (log or chk)
  - Linux basics (screen, simple bash scripting)
  - Output (orbitals and surfaces)
  - Time vs. accuracy

(2) Optimizing structures; predicting IR/ Raman
(3) Finding transition states
  - S_N2 (TS-Berny or Scan)
  - Diels-Alder (QTS2)
  - C_3H_5F H shift (QTS3)
(4) Time-Dependant DFT and UV-Vis Spectra
(5) Directing Effects in Electrophilic Aromatic Substitution
(6) Reactions involving a radical ($CH_3^{\bullet} + C_2H_4$)
(7) Solvation and solution chemistry (CH_3-CO-OCH_3 hydrolysis)
Students will choose one of Experiments 6 and 7.

Laboratory – Date, Time, Place

Place: Machray Hall 108
Date and Time: T 2:30-5:25pm
Start: Jan. 14, 20

Resources for those with special needs

- Academic Learning Center, 201 Tier Building, (204)480-1481.
  Website: http://umanitoba.ca/student/academiclearning/
- Student Accessibility Services, 155 University Center, (204)474-6213, (204)474-9790 (TTY).
  Website: http://umanitoba.ca/student/saa/accessibility/
- Student Counselling, 474 University Center, (204)474-8592.
  Website: http://umanitoba.ca/student/counselling/
- University Health Services, 104 University Centre, (204)474-8411
  Website: http://umanitoba.ca/student/health/

Notice Regarding Collection, Use, and Disclosure of Personal Information by the University

Your personal information is being collected under the authority of The University of Manitoba Act. It will be used for the purposes of grading papers and providing feedback to students. Personal information will not be used or disclosed for other purposes, unless permitted by The Freedom of Information and Protection of Privacy Act (FIPPA). The University of Manitoba has taken steps to ensure that its agreement with Crowdmark, Inc. for services provided by the Crowdmark application is in compliance with FIPPA. Please be aware that information held by Crowdmark Inc. may be transmitted to and stored on servers outside of the University of Manitoba, or Canada. The University of Manitoba cannot and does not guarantee protection against the possible disclosure of your data including, without limitation, against possible secret disclosures of data to a foreign authority in accordance with the laws of another jurisdiction. If you have any questions about the collection of personal information, contact the Access and Privacy Office (tel. 204-474-9462), The University of Manitoba, 233 Elizabeth Dafoe Library, Winnipeg, Manitoba, Canada, R3T 2N2.

Appeals

- If you have concerns or questions about posted scores, examination problems, and/or answer keys, promptly consult your instructor.
- No appeals of term work (laboratory, assignment, or mid-term examination grades) will be considered by the course and laboratory coordinators after the final examination has been written.
- If you are not satisfied with the outcome of an appeal regarding term work addressed by the course coordinator or the laboratory coordinator, you can appeal a grade for term work through the Registrar's office. A fee is charged for each appeal. For more information see:
  http://umanitoba.ca/student/records/grades/690.html
- To appeal your final grade, you can initiate the process at the Registrar's office. A fee will be charged for each appeal. For more information, see:
  http://umanitoba.ca/student/records/

Limited Access and VW Resources

Students who fail or VW from a course will be subject to limited access to that course in future terms. That is, students will not be able to register for a course (for which they have VWed or failed) during the limited access registration period. For more information, please see the Repeated Course policy available at:
http://www.umanitoba.ca/admin/governance/media/Repeated_Course_Policy_-_2016_09_01.pdf

Academic integrity policies

Plagiarism

Copying another student's examination, laboratory reports, or assignments, or an instructor's answer sheet from a previous year is plagiarism. If you quote other sources of information in a laboratory report or other assignment, you must give proper credit. Plagiarism and other forms of cheating are prohibited. The full definition of plagiarism and the possible penalties associated with it are outlined in the General Calendar of the University.

Cheating

The possession of unauthorized materials during an examination, including "crib notes" (whether hand-written or contained within a computer/calculator), is considered cheating and subject to action by the Student Disciplinary By-Law. Only calculators are permitted in an examination – no texts, notes, dictionaries, etc. Students found with cell phones, pagers, text in their calculators or other unauthorized material within their reach during a chemistry examination will be given a grade of zero (0) on that examination and further penalties may apply.

Faculty of science statement on academic dishonesty

The Faculty of Science and The University of Manitoba regard acts of academic dishonesty in quizzes, tests, examinations, laboratory reports or assignments as serious offences and may assess a variety of penalties depending on the nature of the offence. Acts of academic dishonesty include, but are not limited to, bringing unauthorized materials into a test or exam, copying from another individual, using answers provided by tutors, plagiarism, and examination impersonation. **Cell phones, pagers, PDAs, MP3 units or electronic translators are explicitly listed as unauthorized materials, and must *not* be present during tests or examinations.**

Penalties that may apply, as provided for under the University of Manitoba's Student Discipline By-Law, range from a grade of zero for the assignment or examination, failure in the course, to expulsion from the University.

The Student Discipline By-Law may be accessed at:

http://umanitoba.ca/admin/governance/governing_documents/students/student_discipline.html

Suggested minimum penalties assessed by the Faculty of Science for acts of academic dishonesty are available on the Faculty of Science Academic Dishonesty Guidelines and Penalties web-page

http://umanitoba.ca/faculties/science/resources/Acad_Dishon_TABLE_RevCSS_AdminC_Jul2012_WEB.pdf

All Faculty members (and their teaching assistants) have been instructed to be vigilant and report all incidents of academic dishonesty to the Head of the Department.

For more definitions, policy details, informative case studies, and an Academic Honesty Quiz see:

http://umanitoba.ca/faculties/science/undergrad/resources/webdisciplinedocuments.html

Copyright and Intellectual Properties Resources

Copyrights and intellectual property must be respected by all students. For more information, please refer to the Copyright Office: http://umanitoba.ca/copyright/

Last but not least: I appreciate input and feedback, both formally and informally!