Computational Chemistry
CHEM 413/ENCH 413
Fall Term, 2021

Monday: 1:30 pm-2:30 pm | Wednesday: 12:30 pm – 1:30 pm | Friday 11:30 am – 12:30 pm

- Monday session is for scheduled one-on-one meetings (e.g., for grading assignments).
- Wednesday session is synchronous (typically hands-on practice).
- Friday is asynchronous (typically the material for next week will be posted).

Instructor: Farnaz Heidar-Zadeh
Instructor Contact Information: farnaz.heidarzadeh@queensu.ca
Office Hours:
> Please send me an email to set a date/time to meet. I will be monitoring the course discussion venue daily to answer any questions or concerns you might have.

1. Course Description
The application of quantum mechanics to chemical structures, energetics, internal motions of molecules, and chemical reactions. An introduction to the use of modern electronic structure software in chemistry.

2. Intended Student Learning Outcomes and methods of assessment
Upon successful completion of this course, students will be able to:
1. Describe the concepts and assumptions underlying various computational chemistry models.
2. Assess the quality and suitability of computational chemistry methods reported in the literature.
3. Be able to determine the suitable method(s) for a specific chemical problem at hand.
4. Perform computational chemistry calculations using commercial and free software packages to calculate properties.
5. Be able to read and write simple Python programs and general scripts for computational chemistry calculations and workflows.

The assignments and one-on-one meetings are designed to test these learning outcomes. Learning outcomes 3 and 5 are especially transferable to other research areas and professional development.

3. Course materials/Readings and timeline.
There is no required textbook for this course. However, the following books may be useful:
1. Essentials of Computational Chemistry: Theories and Models, Christopher Cramer
2. Introduction to Computational Chemistry, Frank Jensen
3. Computational Chemistry, Jeremy Harvey

The (rough) course outline is scheduled as follows:
PART A (First 6 Weeks)
> Topic 01: Introduction to Computational Chemistry
> Topic 02: Python Programming & Scripting
> Topic 03: Potential Energy Surface Landscape
> Topic 04: Molecular Mechanics
> Topic 05: Molecular Dynamics

PART B (Second 6 Weeks)
    Topic 06: Introduction to Quantum Chemistry
    Topic 07: Hartree-Fock Theory
    Topic 08: Post Hartree-Fock Theory
    Topic 09: Density Functional Theory
    Topic 10: Chemical Concepts

6. <u>Grading Scheme</u>

There would be weekly assignments due on Fridays (except for September 10 and October 8 & 15). There is no final exam.

    45%   Assignments
    45%   One-on-one meeting (e.g., for marking assignments)
    10%   Reflection Reports

7. <u>Grading Method</u>

All components of this course will receive numerical percentage marks. The final grade you receive for the course will be derived by converting your numerical course average to a letter grade according to Queen's Official Grade Conversion Scale:

Queen's Official Grade Conversion Scale

Grade	Numerical Course Average (Range)
A+	90-100
A	85-89
A-	80-84
B+	77-79
B	73-76
B-	70-72
C+	67-69
C	63-66
C-	60-62
D+	57-59
D	53-56
D-	50-52
F	49 nd below

8. <u>Late Policy</u>

If you require additional time to complete an assignment, please contact the instructor as soon as possible. See below for the Chemistry Department policy on *missed* quizzes, tests, midterms, presentations, and assignments:
https://www.chem.queensu.ca/undergraduate/undergraduate-resources/missed-exam-policy

9. <u>Location and Timing of Final Examinations</u>

There is no final exam for this course.

10. <u>Academic Integrity</u>

Please refer to the course website on onQ and check "University and Course Policies".

11. **Technology**
    General course technology requirements are listed below. For synchronous sessions and office hours, it would be preferred if the student has access to a headset and webcam.

    Web Browsers: onQ performs best when using the most recent version of the web browsers, Chrome or Firefox. Safari and Edge are strongly discouraged as these web browsers are known to cause issues with onQ.

    Internet Speed: While wired internet connection is encouraged, we recognize that students may be relying on a wireless connection. A minimum download speed of 10 Mbps and up to 20 Mbps for multimedia is recommended. To test your internet speed, https://www.speedtest.net/

    For technology support ranging from setting up your device, issues with onQ to installing software, contact ITS Support Centre https://www.queensu.ca/its/itsc

12. **Copyright of Course Materials**
    Please refer to the course website on onQ and check "University and Course Policies".

13. **Privacy Statement for Instructors Who Use External Software in Their Course**
    This course makes use of Turnitin. Please refer to the course website on onQ and check "University and Course Policies".

    This course will also use external software, including Jupyter notebooks, Anaconda, and WebMO. Your use of these tools is subject to the terms of use and privacy policies imposed by their providers. If, upon review of the terms imposed by these packages you have concerns, please contact the instructor.

14. **Notice of Recording**
    Synchronous (live) classes will be delivered in this course through a video conferencing platform supported by the University MS Teams or Zoom. Steps have been taken by the University to configure these platforms in a secure manner. Classes will be recorded with video and audio (and in some cases transcription) and will be made available to students in the course for the duration of the term. The recordings may capture your name, image or voice through the video and audio recordings. By attending these live classes, you are consenting to the collection of this information for the purposes of administering the class and associated coursework. If you are concerned about the collection of your name and other personal information in the class, please contact the course instructor to identify possible alternatives.
    To learn more about how your personal information is collected, used and disclosed by Queen's University, please see the general Notice of Collection, Use and Disclosure of Personal Information

15. **Accommodations for Disabilities**
    Please refer to the course website on onQ and check "University and Course Policies".

16. **Academic Considerations for Students in Extenuating Circumstances**
    Queen's University is committed to providing academic consideration to students experiencing extenuating circumstances that are beyond their control and are interfering with their ability to complete academic requirements related to a course for a short period of time. The Senate Policy on Academic Consideration for Students in Extenuating Circumstances is available at:

http://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslcwww/files/files/policies/senateandtrustees/Academic%20Considerations%20for%20Extenuating%20Circumstances%20Policy%20Final.pdf

Each Faculty has developed a protocol to provide a consistent and equitable approach in dealing with requests for academic consideration for students facing extenuating circumstances. Arts and Science undergraduate students can find the Faculty of Arts and Science protocol and the portal where a request can be submitted at: http://www.queensu.ca/artsci/accommodations. Students in other Faculties and Schools who are enrolled in this course should refer to the protocol for their home Faculty.

If you need to request academic consideration for this course, you will be required to provide the name and email address of the instructor/coordinator.

17. **Discussion Guidelines**
   University is a place to share, question and challenge ideas. Each student brings a different lived experience from which to draw upon. To help one another learn the most we can from this experience please consider the following   guidelines.

   1. Make a personal commitment to learn about, understand, and support your peers.
   2. Assume the best of others and expect the best of them.
   3. Acknowledge the impact of oppression on the lives of other people and make sure your writing is respectful and inclusive.
   4. Recognize and value the experiences, abilities, and knowledge each person brings.
   5. Pay close attention to what your peers write before you respond. Think through and re-read your writings before you post or send them to others.
   6. It's ok to disagree with ideas, but do not make personal attacks.
   7. Be open to being challenged or confronted on your ideas and to challenging others with the intent of facilitating growth. Do not demean or embarrass others.
   8. Encourage others to develop and share their ideas.