*We recognize and acknowledge that McMaster University meets and learns on the traditional territories of the Mississauga and Haudenosaunee nations, and within the lands protected by the “Dish With One Spoon” wampum, an agreement amongst all allied Nations to peaceably share and care for the resources around the Great Lakes.*

**CHEM 4PB3 – Computational Models for Electronic Structure and Chemical Bonding**

# 2022 Winter Term

**Instructor:**  Rodrigo A. Vargas-Hernández |  **E-mail:** [vargashr@mcmaster.ca](mailto:vargashr@mcmaster.ca) | **Office:** ABB 266

## Course Description

With the rise of cloud computing and open-source code, chemists rely more on modern tools to accelerate their research.

This course will serve as an introduction to the principles and application of the computational toolbox for in silico prediction of the structures and properties of new compounds and materials. The course will be a seminar-style class that combines an introduction to electronic structure methods (first half) and machine learning algorithms (second half).

The tools covered in the course will allow the student to model and study material with target properties, e.g., particular band gap, predicting binding constants of small molecules or a reaction mechanism.

## Course and Learning Objectives

The “obvious” objective is for the students to learn and be familiar with modern computational tools to study and simulate molecular systems. The more subtle, important, and difficult objective is being more familiar with modern software and numerical tools.

By the end of this course, the student will hopefully be more capable of using packages needed to understand chemistry.

## Make-up and Attendance policy

The primary element of the course is the final project. My intention is to assess assignments and the final project in person. Attending lectures/tutorials is not essential, but the final presentation in person is mandatory.

Marks will reflect not only the correctness of the answer but the depth of insight that led to the answer.

## Materials & Fees

### Required Materials/ Resources

* Materials will be posted the course web site, **<ADD LINK>**, including the textbooks, papers, and tutorials. I do not follow any book closely, and the documents, notebooks, and videos I put online are the authoritative reference for the course.

## Delivery (to be determined) (CHECK THIS!!)

**It is intended that the course will be delivered in person.** If online delivery is required, you will require a computer that meets theperformance requirements [found here](https://cto.mcmaster.ca/technology-resources-for-mcmaster-students/#tab-content-device-recommendations).

**Lecture:** Mondays, 2:30-5:30 (HH 305)

**Tutorial:** Tuesdays, 2:30-3:20 (HH 305)

**Office hours:** Tuesday: 3:30-5:30 [However, in general I will stay in my office as long as necessary.]

## Course Overview and Assessment

### Course Outline: - My tentative plan is below.

Quantum chemistry

1. Introduction to Python, GoogleColab, etc.
2. Review of linear algebra
3. Quantum chemistry methods,
   1. Hartree-Fock Theory
   2. Density functional theory
4. Polyatomic systems
5. Potential energy surface
6. Molecular dynamics
7. Force fields and molecular dynamics

Machine learning

1. Linear regression and gradient descent
2. Molecular feature representation
3. Clustering algorithms (unsupervised learning)
4. Neural network
5. Bayesian optimization

This is an absurd amount of material. We will move quickly. Do not get behind. If (when) I wish to modify the schedule/content, I will notify you in class and/or online.

The marking scheme for the course will be primarily based on the final project.

## Make-up and Attendance policy

Attendance is not required. But it is your responsibility to attend office hours or other dedicated sessions for your assessments to be graded.

## General Remarks/Advice

It is more important to have the “right ideas” than it is to get the “right answer.” In a course such as this one, it is more important to “think correctly” and “explore new ideas” rather than “follow protocols to reproduce numbers”. Partial credit will often be given when you understand a problem and will always be given when you understand how to solve a problem.

**Don’t get behind**. The volume of material in this course is staggering. It will require a daily commitment from you. Probably most of you are smart enough so that you have been able to get by studying just the night before the test. That ends here. You will need to read and take notes on the book before class. After

class, you will need to go through the lecture notes, rewriting them and adding marginal comments/questions about the material. Then you will need to work through some of the problems in the book and think critically about the material. This course will probably require a larger commitment of time and mental energy than any course you have ever taken before.

After the pandemic there was an increment in online material/tutorials of some of the topics that we will cover, I encourage to take advantage of those. Exploring and being more familiar with computational tools will only benefit your future career.

**Ask questions**. Please visit me during office hours. (I get lonely.) I will clarify points in lecture that were not clear (sorry!), provide guidance on the final project and class exercises/examples. More generally, I will do everything in my power to try to help you through this course.

**Don’t be afraid** to criticize/comment on the course. In general, my teaching methods are flexible, and I will adapt them to your needs; my goal is for you to learn the material of the course. I’ve designed this course based on what my opinions of what will work. I expect to change things during the term based on feedback and suggestions from you. I’m even open to totally including new material on the fly, if I believe is more relevant for your final project. Thus, it is important that you make suggestions and/or tell me about portions of the course that need improvement. (Even if I do not agree with your suggestion, I will try to come up with an alternative approach that addresses your concerns.) If you feel uncomfortable giving feedback in person, slide a note under my door, get someone else to talk to me on your behalf (preserving your anonymity, if you wish), or come and talk to me yourself but raise your concerns in the third person: for example, “I don’t feel this way, but some of the people in class think your lectures are about as exciting as watching ice sublime.”

**Learn good study skills**.

Humans as opposed to machine learning models are good at generalizing a problem across different tasks. Since there isn’t an exam, I expect the students to dedicate enough time to understand the range of applicability of some of the topics we will cover in the course. Studding is not memorizing a material, that approach will not work in this course.

My tips for managing this course are:

1. Prepare for lectures beforehand. Review the notes from the previous lecture and read the relevant sections. [30 minutes/class]
2. Take advantage of additional online material.
3. Take notes
4. Review lectures afterwards.
5. Do not be afraid of coding and asking questions.
6. Work example problems. [4 hours/week]
7. Think critically about the material. Try to imagine why a topic we covered in class is useful and where it might be applied. Therefore, the emphasis in the final project. [~2 hours/week]

## Rodrigo’s Draconian Academic Integrity Policy

I have absolutely no tolerance for cheating. I believe hard effort pays off. The final project will have fingerprints of you all over it, from the chosen problem to the final presentation.

For the final project, each group must state what was developed and what tools were used, meaning recognizing someone else’s work that was used in the project.

If you have inadvertently (or even purposely) engaged in impermissible collaboration, you should come to me. Together we will work out a remedy that is fair to you and the rest of the class. If I catch you cheating, you have up to 48 hours to come to me and confess your transgression. If you do not raise the matter of your own accord, I will check with the appropriate Dean and if it is your first offense, you will fail the course. This will be registered as your “first offense” with the Dean. If it is your second offense, then the matter will be referred to the faculty council and I will argue forcibly that you should receive a zero for the course and that your behavior should become part of your permanent academic record. See <http://www.mcmaster.ca/policy/academic.htm>.

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# Policies and **Procedures –** (McMaster’s Official Legalese)

## Requests for Relief for Missed Academic Term Work

[McMaster Student Absence Form (MSAF):](https://secretariat.mcmaster.ca/university-policies-procedures-guidelines/msaf-mcmaster-student-absence-form/) In the event of an absence for medical or other reasons, students should review and follow the Academic Regulation in the Undergraduate Calendar “Requests for Relief for Missed Academic Term Work”.

### MSAF Course Specific Information

I will not give make-up assignments. If you know you will miss an assignment you must arrange it with me beforehand.

## Academic Accommodation of Students with Disabilities

Students with disabilities who require academic accommodation must contact [Student Accessibility Services (SAS](https://sas.mcmaster.ca/)) at 905-525-9140 ext. 28652 or [sas@mcmaster.ca](mailto:sas@mcmaster.ca) to make arrangements with a Program Coordinator. For further information, consult McMaster University’s [*Academic Accommodation of Students with Disabilities*](https://secretariat.mcmaster.ca/app/uploads/Academic-Accommodations-Policy.pdf) policy.

I will work with students with documented disabilities, and more generally with students who have temporary disabilities or other factors that inhibit their ability to perform at a high level. My goal is be maximally supportive of my students, and to treat everyone fairly. This means that while I am eager to accommodate all of you, I hold the same high expectations for all of you.

## Academic Accommodation for Religious, Indigenous Or Spiritual Observances (Riso)

Students requiring academic accommodation based on religious, indigenous or spiritual observances should follow the procedures set out in the [RISO](https://secretariat.mcmaster.ca/app/uploads/2019/02/Academic-Accommodation-for-Religious-Indigenous-and-Spiritual-Observances-Policy-on.pdf) policy. Students should submit their request to their Faculty Office ***normally within 10 working days*** of the beginning of term in which they anticipate a need for accommodation or to the Registrar's Office prior to their examinations. Students should also contact their instructors as soon as possible to make alternative arrangements for classes, assignments, and tests.

## Courses with An On-Line Element

***Some courses*** ***may*** use on-line elements (e.g. e-mail, Avenue to Learn (A2L), LearnLink, web pages, capa, Moodle, ThinkingCap, etc.). Students should be aware that, when they access the electronic components of a course using these elements, private information such as first and last names, user names for the McMaster e-mail accounts, and program affiliation may become apparent to all other students in the same course. The available information is dependent on the technology used. Continuation in a course that uses on-line elements will be deemed consent to this disclosure. If you have any questions or concerns about such disclosure, please discuss this with the course instructor.

## Online Proctoring

***Some courses may*** use online proctoring software for tests and exams. This software may require students to turn on their video camera, present identification, monitor and record their computer activities, and/or lock/restrict their browser or other applications/software during tests or exams. This software may be required to be installed before the test/exam begins.

## Academic Integrity

You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity.

**It is your responsibility to understand what constitutes academic dishonesty.**

Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: “Grade of F assigned for academic dishonesty”), and/or suspension or expulsion from the university. For information on the various types of academic dishonesty please refer to the [*Academic Integrity Policy*](https://secretariat.mcmaster.ca/app/uploads/Academic-Integrity-Policy-1-1.pdf)*,* located at [https://secretariat.mcmaster.ca/university-policies-procedures- guidelines/](https://secretariat.mcmaster.ca/university-policies-procedures-%20guidelines/)

**The following illustrates only three forms of academic dishonesty:**

* plagiarism, e.g. the submission of work that is not one’s own or for which other credit has been obtained.
* improper collaboration in group work.
* copying or using unauthorized aids in tests and examinations.

## Authenticity / Plagiarism Detection

***Some courses may*** use a web-based service (Turnitin.com) to reveal authenticity and ownership of student submitted work. For courses using such software, students will be expected to submit their work electronically either directly to Turnitin.com or via an online learning platform (e.g. A2L, etc.) using plagiarism detection (a service supported by Turnitin.com) so it can be checked for academic dishonesty.

Students who do not wish their work to be submitted through the plagiarism detection software must inform the Instructor before the assignment is due. No penalty will be assigned to a student who does not submit work to the plagiarism detection software. **All submitted work is subject to normal verification that standards of academic integrity have been upheld** (e.g., on-line search, other software, etc.). For more details about McMaster’s use of Turnitin.com please go to the [McMaster Office of Academic Integrity](https://www.mcmaster.ca/academicintegrity/)’s webpage.

## Conduct Expectations

As a McMaster student, you have the right to experience, and the responsibility to demonstrate, respectful and dignified interactions within all our living, learning and working communities. These expectations are described in the [*Code of Student Rights & Responsibilities* (the “Code”).](https://secretariat.mcmaster.ca/app/uploads/Code-of-Student-Rights-and-Responsibilities.pdf) All students share the responsibility of maintaining a positive environment for the academic and personal growth of all McMaster community members, **whether in person or online**.

It is essential that students be mindful of their interactions online, as the Code remains in effect in virtual learning environments. The Code applies to any interactions that adversely affect, disrupt, or interfere with reasonable participation in University activities. Student disruptions or behaviours that interfere with university functions on online platforms (e.g. use of Avenue 2 Learn, WebEx or Zoom for delivery), will be taken very seriously and will be investigated. Outcomes may include restriction or removal of the involved students’ access to these platforms.

## Copyright and Recording

Students are advised that lectures, demonstrations, performances, and any other course material provided by an instructor include copyright protected works. The Copyright Act and copyright law protect every original literary, dramatic, musical and artistic work, **including lectures** by University instructors.

The recording of lectures, tutorials, or other methods of instruction may occur during a course. Recording may be done by either the instructor for the purpose of authorized distribution, or by a student for the purpose of personal study. Students should be aware that their voice and/or image may be recorded by others during the class. Please speak with the instructor if this is a concern for you.

**Research Ethics** -NA

## Extreme Circumstances

The University reserves the right to change the dates and deadlines for any or all courses in extreme circumstances (e.g., severe weather, labour disruptions, etc.). Changes will be communicated through regular McMaster communication channels, such as McMaster Daily News, A2L and/or McMaster email.