



COURSE OUTLINE

1. **Course:** CHEM 373, Physical Chemistry: Quantum Chemistry - Fall 2023

Coordinator(s)

Name	Email	Phone	Office	Hours
Dr. Max Anikovskiy	m.anikovskiy@ucalgary.ca	403 220-3115	EEEL 237A	by appointment

Section(s)

Lecture 01 : TR 12:30 - 13:45 in ST 145

Instructor	Email	Phone	Office	Hours
Dr. Max Anikovskiy	m.anikovskiy@ucalgary.ca	403 220-3115	EEEL 237A	by appointment

To account for any necessary transition to remote learning for the current semester, courses with in-person lectures, labs, or tutorials may be shifted to remote delivery for a certain period of time. In addition, adjustments may be made to the modality and format of assessments and deadlines, as well as to other course components and/or requirements, so that all coursework tasks are in line with the necessary and evolving health precautions for all involved (students and staff).

In Person Delivery Details:

All class components including lectures, labs, and tutorials will be delivered in person.

Course Site:

D2L: CHEM 373 L01-(Fall 2023)-Physical Chemistry: Quantum Chemistry

Note: Students must use their U of C account for all course correspondence.

Equity Diversity & Inclusion:

The University of Calgary is committed to creating an equitable, diverse and inclusive campus, and condemns harm and discrimination of any form. We value all persons regardless of their race, gender, ethnicity, age, LGBTQIA2S+ identity and expression, disability, religion, spirituality, and socioeconomic status. The Faculty of Science strives to extend these values in every aspect of our courses, research, and teachings to better promote academic excellence and foster belonging for all.

The Chemistry EDI Committee acknowledges there are persistent barriers that prevent such accessibility and hinder our progress towards EDI. Our representatives (faculty, postdocs, graduate and undergraduate students) are committed to addressing any concerns and work towards proactive solutions that enact necessary change within the department. To submit anonymous questions, comments or concerns regarding EDI related issues, please reach out to our Associate Head EDI, Belinda Heyne (bjmheyne@ucalgary.ca)

2. **Requisites:**

See section [3.5.C](#) in the Faculty of Science section of the online Calendar.

Prerequisite(s):

Chemistry 201 or 211; and 203 or 213; Physics 223 or 355; Mathematics 267 or 277.

3. **Grading:**

The University policy on grading and related matters is described in [F.1](#) and [F.2](#) of the online University Calendar.

In determining the overall grade in the course the following weights will be used:

Course Component	Weight	Due Date (duration for exams)	Modality for exams	Location for exams
Laboratory (5) ¹	25%	Ongoing		
Tutorials (11) ²	22%	Ongoing		
Midterm	18%	Nov 02 2023 at 12:30 pm (75 Minutes)	in-person	In class
Registrar Scheduled Final Exam	35%	Will be available when the final exam schedule is released by the Registrar	in person	Will be available when the final exam schedule is released by the Registrar

¹ A total of 5 laboratory exercises will be graded. All laboratory exercises have the same weight. A pre-laboratory quiz administered by a teaching assistant in the laboratory at the beginning of each lab session must be completed in order for a student to be able to attempt the laboratory exercise. The pre-laboratory quizzes have the same weight and are worth 30% of the laboratory component grade. Although all laboratory exercises are expected to be completed during the lab session, a buffer period until 11:59 pm on the next day after lab will be provided for submitting the lab reports. The reports are to be uploaded to a designated Dropbox on D2L.

² A total of 11 tutorial quizzes will be graded. All tutorial quizzes will have the same weight. The quizzes will be administered through D2L and become available after tutorial. If a written response is required, the file in either a .pdf or .docx format is to be submitted to a designated D2L Dropbox. The submission deadline is 11:59 pm on the next day after tutorial.

Each piece of work (reports, assignments, quizzes, midterm exam(s) or final examination) submitted by the student will be assigned a grade. The student's grade for each component listed above will be combined with the indicated weights to produce an overall percentage for the course, which will be used to determine the course letter grade.

The conversion between a percentage grade and letter grade is as follows.

	A+	A	A-	B+	B	B-	C+	C	C-	D+	D
Minimum % Required	95 %	86 %	82 %	78%	74%	70 %	66 %	62%	58%	54 %	50 %

This course will have a Registrar Scheduled Final exam that will be delivered in-person and on campus. [The Final Examination Schedule](#) will be published by the Registrar's Office approximately one month after the start of the term. The final exam for this course will be designed to be completed within 3 hours.

In order to pass this course with a letter grade higher than a D+, ALL of the following requirements must be met:

1. A passing grade for the weighted average of the midterm and final examination.
2. A passing grade for the laboratory component of the course.
3. Completion of a minimum of 9 tutorial quizzes.
4. Completion of a minimum of 4 laboratory exercises.

The University of Calgary offers a [flexible grade option](#), Credit Granted (CG) to support student's breadth of learning and student wellness. Faculty units may have additional requirements or restrictions for the use of the CG grade at the faculty, degree or program level. To see the full list of Faculty of Science courses where CG is not eligible, please visit the following website: <https://science.ucalgary.ca/current-students/undergraduate/program-advising/flexible-grading-option-cg-grade>

4. Missed Components Of Term Work:

In the event that a student legitimately fails to submit any online or in-person assessment on time (e.g. due to illness, domestic affliction, etc...), please contact the course coordinator, or the course instructor if this course does not have a coordinator to arrange for a re-adjustment of a submission date, or possible exemption and reweighing of components. Absences not reported within 48 hours will not be accommodated. Students may be asked to provide supporting documentation ([Section M.1](#)) for an excused absence, See [FAQ](#).

If an excused absence is approved, options for how the missed assessment is dealt with is at the discretion of the coordinator or course instructor. Some options such as an exemption and pro-rating among the components of the course may not be a viable option based on the design of this course.

There is no deferred midterm examination in this class. In the event that a student misses the midterm and an excused absence is approved, the weight of the midterm examination will be shifted to the final examination.

In the event that a student misses a laboratory activity and an excused absence is approved, a make up lab will be scheduled. If there is no possibility to schedule a make up lab, the weight of the missed laboratory experiment will be pro-rated among the remaining lab component.

5. **Scheduled Out-of-Class Activities:**

There are no scheduled out of class activities for this course.

6. **Course Materials:**

Recommended Textbook(s):

Thomas Engel and Philip Reid, *Physical Chemistry: Quantum Chemistry*: Pearson.

In order to successfully engage in their learning experiences at the University of Calgary, students taking online, remote and blended courses are required to have reliable access to the following technology:

- A computer with a supported operating system, as well as the latest security, and malware updates;
- A current and updated web browser;
- Webcam/Camera (built-in or external);
- Microphone and speaker (built-in or external), or headset with microphone;
- Current antivirus and/or firewall software enabled;
- Stable internet connection.

For more information please refer to the UofC [ELearning](#) online website.

7. **Examination Policy:**

Examinations will be closed book. Non-programmable calculators during examinations will be allowed. Calculator Feature: the capability to perform calculations electronically on user-entered numerical data without the capability to employ pre-stored or user-entered formulae. This feature is provided by the most elementary calculator, permits the elementary arithmetic operations (addition, subtraction, multiplication and division) and possibly the trigonometric, hyperbolic, exponential and logarithmic operations.

Students should also read the Calendar, [Section G](#), on Examinations.

8. **Approved Mandatory And Optional Course Supplemental Fees:**

There are no mandatory or optional course supplemental fees for this course.

9. **Writing Across The Curriculum Statement:**

For all components of the course, in any written work, the quality of the student's writing (language, spelling, grammar, presentation etc.) can be a factor in the evaluation of the work. See also Section [E.2](#) of the University Calendar.

In this course, the quality of the student's writing in all submitted work will be a factor in the evaluation of this work. See also Section E.2 of the University Calendar.

10. **Human Studies Statement:**

Students will not participate as subjects or researchers in human studies.

See also [Section E.5](#) of the University Calendar.

11. **Reappraisal Of Grades:**

A student wishing a reappraisal, should first attempt to review the graded work with the Course coordinator/instructor or department offering the course. Students with sufficient academic grounds may request a reappraisal. Non-academic grounds are not relevant for grade reappraisals. Students should be aware that the grade being reappraised may be raised, lowered or remain the same. See [Section I.3](#) of the University Calendar.

- Term Work:** The student should present their rationale as effectively and as fully as possible to the Course coordinator/instructor within **ten business days** of either being notified about the mark, or of the item's return to the class. If the student is not satisfied with the outcome, the student shall submit the Reappraisal of Graded Term work [form](#) to the department in which the course is offered within 2 business days of receiving the decision from the instructor. The Department will arrange for a reappraisal of the work within the next ten business days. The reappraisal will only be considered if the student provides a detailed rationale that outlines where and for what reason an error is suspected. See sections [I.1](#) and [I.2](#) of the University Calendar
- Final Exam:** The student shall submit the request to Enrolment Services. See [Section I.3](#) of the University Calendar.

12. Other Important Information For Students:

- a. **Mental Health** The University of Calgary recognizes the pivotal role that student mental health plays in physical health, social connectedness and academic success, and aspires to create a caring and supportive campus community where individuals can freely talk about mental health and receive supports when needed. We encourage you to explore the mental health resources available throughout the university community, such as counselling, self-help resources, peer support or skills-building available through the SU Wellness Centre (Room 370, MacEwan Student Centre, [Mental Health Services Website](#)) and the Campus Mental Health Strategy website ([Mental Health](#)).
- b. **SU Wellness Services:** For more information, see their [website](#) or call [403-210-9355](#).
- c. **Sexual Violence:** The Sexual Violence Support Advocate, Carla Bertsch, can provide confidential support and information regarding sexual violence to all members of the university community. Carla can be reached by email (syva@ucalgary.ca) or phone at [403-220-2208](#). The complete University of Calgary policy on sexual violence can be viewed [here](#).
- d. **Student Ombuds Office:** A safe place for all students of the University of Calgary to discuss student related issues, interpersonal conflict, academic and non-academic concerns, and many other problems.
- e. **Student Union Information:** [SU contact](#), Email your SU Science Reps: science1@su.ucalgary.ca, science2@su.ucalgary.ca, science3@su.ucalgary.ca,

f. Academic Accommodation Policy:

It is the student's responsibility to request academic accommodations according to the University policies and procedures listed below. The student accommodation policy can be found at: <https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Student-Accommodation-Policy.pdf>

Students needing an accommodation because of a disability or medical condition should communicate this need to Student Accessibility Services in accordance with the Procedure for Accommodations for Students with Disabilities: <https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Accommodation-for-Students-with-Disabilities-Procedure.pdf>.

Students needing an accommodation in relation to their coursework or to fulfil requirements for a graduate degree, based on a Protected Ground other than Disability, should communicate this need, by filling out the [Request for Academic Accommodation Form](#) and sending it to Associate Head, Undergraduate by email ahugchem@ucalgary.ca preferably 10 business days before the due date of an assessment or scheduled absence.

- g. **Misconduct:** Academic integrity is the foundation of the development and acquisition of knowledge and is based on values of honesty, trust, responsibility, and respect. We expect members of our community to act with integrity. Research integrity, ethics, and principles of conduct are key to academic integrity. Members of our campus community are required to abide by our institutional [Code of Conduct](#) and promote academic integrity in upholding the University of Calgary's reputation of excellence. Some examples of academic misconduct include but are not limited to: posting course material to online platforms or file sharing without the course instructor's consent; submitting or presenting work as if it were the student's own work; submitting or presenting work in one course which has also been submitted in another course without the instructor's permission; borrowing experimental values from others without the instructor's approval; falsification/fabrication of experimental values in a report. Please read the following to inform yourself more on academic integrity:

[Student Handbook on Academic Integrity](#)
[Student Academic Misconduct Policy](#) and [Procedure](#)
[Faculty of Science Academic Misconduct Process](#)
[Research Integrity Policy](#)

Additional information is available on the [Student Success Centre Academic Integrity page](#)

- h. **Copyright of Course Materials:** All course materials (including those posted on the course D2L site, a course website, or used in any teaching activity such as (but not limited to) examinations, quizzes, assignments, laboratory manuals, lecture slides or lecture materials and other course notes) are protected by law. These materials are for the sole use of students registered in this course and must not be redistributed. Sharing these materials with anyone else would be a breach of the terms and conditions governing student access to D2L, as well as a violation of the copyright in these materials, and may be pursued as a case of student academic or [non-academic misconduct](#), in addition to any other remedies available at law.
- i. **Freedom of Information and Privacy:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPP). Students should identify themselves on all written work by

placing their name on the front page and their ID number on each subsequent page. For more information, see [Legal Services](#) website.

- j. **Surveys:** At the University of Calgary, feedback through the Universal Student Ratings of Instruction ([USRI](#)) survey and the Faculty of Science Teaching Feedback form provides valuable information to help with evaluating instruction, enhancing learning and teaching, and selecting courses. Your responses make a difference - please participate in these surveys.

Course Outcomes:

- Recognize the limitations of classical theory; name postulates upon which the quantum theory is built.
- Explain the structure of the Schrödinger equation and solve the equation for model and real world systems; recognize the connection between operators and observables; evaluate probability amplitudes and expectation values.
- Apply approximation techniques to solving quantum chemical problems.
- Explain electronic and energy configuration of atoms and molecules using quantum chemical approaches.
- Gain skills in solving quantum chemical problems using computational methods.

Electronically Approved - Aug 28 2023 12:57

Department Approval