

## Quantum Mechanics CHEM/ENCH 313

Instructor: Tucker Carrington

### Instructor Contact Information

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Office Hours: on request, any time, by zoom. Send me an email to arrange a time.

TA: Sangeeth D. Kallullathil

### TA Contact Information:

Email: sdk4@queensu.ca

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### Intended Student Learning Outcomes

At the end of CHEM/ENCH 313, students will be able to:

- Explain the postulates and general principles of quantum mechanics.
- Solve the Schrödinger equation for systems such as the particle in a box, harmonic oscillator, rigid rotor, and the Hydrogen atom.
- Apply the variational method and perturbation theory to chemical systems.
- Apply quantum mechanics to describe the electronic structure of molecules and calculate molecular properties.
- Provide a quantum-mechanical description for chemical concepts such as atomic and molecular orbitals.

### Course Outline

- i) The Postulates of Quantum Mechanics: The Schrödinger equation, wavefunctions, expectation values, Ehrenfest's theorem
- ii) Applications to Simple Problems: the free particle and wave packets, 1D and 3D square infinite wells, the harmonic oscillator, the rigid rotor, the hydrogen atom
- iii) Approximation Methods: perturbation theory, the variational method
- iv) Multielectron Systems: Hartree-Fock and CI methods, Hückel method
- v) Molecules: the Born-Oppenheimer approximation
- vi) Time dependent problems: Absorption of radiation, inelastic scattering

### Textbooks

Reference book: Quantum Chemistry, Donald A. McQuarrie, 2<sup>nd</sup> edition

Additional reading: Quantum Chemistry, Ira N. Levine, 7<sup>th</sup> edition

Both books are available in the library.

### Marking Scheme

**EVALUATION:**

First midterm: 20%

Second midterm: 20%

Three assignments: 12%

Final exam 48%

**PROPOSED DATES:****First assignment due at the end of the lecture on the 23<sup>rd</sup> of September****First midterm during the lecture on the 8<sup>th</sup> of October****Second assignment due the 21<sup>st</sup> of October****Second midterm during the lecture on the 12<sup>th</sup> of November****Third assignment due the 25<sup>th</sup> of November**

All components of this course will receive letter grades which, for purposes of calculating your course average, will be translated into numerical equivalents using the Faculty of Arts and Science approved scale (see below). Your course average will then be converted to a final letter grade according to Queen's Official Grade Conversion Scale (see below).

***Arts & Science Letter Grade Input Scheme***

Assignment mark	Numerical value for calculation of final mark
A+	93
A	87
A-	82
B+	78
B	75
B-	72
C+	68
C	65
C-	62
D+	58
D	55
D-	52
F48 (F+)	48
F24 (F)	24
FO (O)	0

***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 and below

#### **4. Timing of Final Examinations**

The exam dates for each Term are listed on the Faculty of Arts and Science webpage under “[Important Dates](#).” Student exam schedules for the Fall Term are posted via SOLUS immediately prior to the Thanksgiving holiday. **Students should delay finalizing any travel plans until after the examination schedule has been posted. Exams will not be moved or deferred to accommodate employment, travel/holiday plans or flight reservations.**

#### **Remote Exams**

For exams being offered remotely, Regulation 7.2.3. [Restrictions on Assessment](#) is waived. Remote exams will be allowed in the last two weeks of classes and in the study period designated by Senate prior to the examination period in order to accommodate the limited number of online proctoring seats available.

#### **Copyright of Course Materials**

Materials generated by instructors of this course, including assignments and quizzes, are copyrighted and may not be shared with anyone other than students registered in this course.

#### **5. Statement on Academic Integrity**

The following statement on academic integrity builds on a definition approved by Senate and is designed to make students aware of the importance of the concept and the potential consequences of departing from the core values of academic integrity. It is highly recommended that this statement be included on all course syllabi. Instructors may also consider including this statement with each assignment.

Queen’s students, faculty, administrators and staff all have responsibilities for upholding the fundamental values of academic integrity; honesty, trust, fairness, respect, responsibility and courage (see [www.academicintegrity.org](http://www.academicintegrity.org)). These values are central to the building, nurturing and sustaining of an academic community in which all members of the community will thrive. Adherence to the values expressed through academic integrity forms a foundation for the "freedom of inquiry and exchange of ideas" essential to the intellectual life of the University (see the Senate Report on Principles and Priorities <http://www.queensu.ca/secretariat/policies/senate/report-principles-and-priorities>).

Students are responsible for familiarizing themselves with the regulations concerning academic integrity and for ensuring that their assignments and their behaviour conform to the principles of academic integrity. Information on academic integrity is available in the Arts and Science Calendar (see Academic Regulation 1 <http://www.queensu.ca/artsci/academic-calendars/regulations/academic-regulations/regulation-1>), on the Arts and Science website (see <https://www.queensu.ca/artsci/students-at-queens/academic-integrity>), and from the instructor of this course. Departures from academic integrity include plagiarism, use of unauthorized materials, facilitation, forgery and falsification, and are antithetical to the development of an academic community at Queen's. Given the seriousness of these matters, actions which contravene the regulation on academic integrity carry sanctions that can range from

a warning or the loss of grades on an assignment to the failure of a course to a requirement to withdraw from the university.

It is recommended that instructors add a paragraph here to explain issues of academic integrity that are particularly relevant to the course. E.g.

- Plagiarism –including guides on how to use sources correctly. Possible example:
  - *Please note that we have had issues in the past with unintended plagiarism in this course. Regardless of how and where you retrieve information, the principles of academic integrity apply. Please visit these helpful websites to help you make sure that you are able to write things in your own words:*
- <https://www.queensu.ca/academicintegrity/students/avoiding-plagiarismcheating>
- <https://integrity.mit.edu/handbook/academic-writing/avoiding-plagiarism-paraphrasing>
- [http://writing.wisc.edu/Handbook/QPA\\_paraphrase.html](http://writing.wisc.edu/Handbook/QPA_paraphrase.html)
- Groupwork-What level of collaboration is acceptable? Clearly state if there are things students must do alone. Possible example:
  - *You are permitted to work with a partner or in groups of 3 to encourage collaboration, cooperation, and collective learning on lab assignments. You are not permitted to share answers among large groups or as a tutorial group. You must work independently on quizzes and ‘pop questions’.*

## **6. Calculator Policy**

As noted in Academic Regulation 9.2, “Calculators acceptable for use during quizzes, tests and examinations are intended to support the basic calculating functions required by most Arts and Science courses. For this purpose, the use of the **Casio 991 series calculator** is permitted and is the only approved calculator for Arts and Science students.”

## **7. Technology**

### **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>

## **Turnitin Statement**

This course makes use of Turnitin, a third-party application that helps maintain standards of excellence in academic integrity. Normally, students will be required to submit their course assignments to through onQ to Turnitin. In doing so, students' work will be included as source documents in the Turnitin reference database, where they will be used solely for the purpose of detecting plagiarism. Turnitin is a suite of tools that provide instructors with information about the authenticity of submitted work and facilitates the process of grading. Turnitin compares submitted files against its extensive database of content, and produces a similarity report and a similarity score for each assignment. A similarity score is the percentage of a document that is similar to content held within the database. Turnitin does not determine if an instance of plagiarism has occurred. Instead, it gives instructors the information they need to determine the authenticity of work as a part of a larger process. Please read Turnitin's Privacy Pledge, Privacy Policy, and Terms of Service, which governs users' relationship with Turnitin. Also, please note that Turnitin uses cookies and other tracking technologies; however, in its service contract with Queen's Turnitin has agreed that neither Turnitin nor its third-party partners will use data collected through cookies or other tracking technologies for marketing or advertising purposes. For further information about how you can exercise control over cookies, see Turnitin's Privacy Policy: Turnitin may provide other services that are not connected to the purpose for which Queen's University has engaged Turnitin. Your independent use of Turnitin's other services is subject solely to Turnitin's Terms of Service and Privacy Policy, and Queen's University has no liability for any independent interaction you choose to have with Turnitin.

## **Accommodations Statement**

Queen's University is committed to achieving full accessibility for persons with disabilities. Part of this commitment includes arranging academic accommodations for students with disabilities to ensure they have an equitable opportunity to participate in all of their academic activities. If you are a student with a disability and think you may need accommodations, you are strongly encouraged to contact Student Wellness Services (SWS) and register as early as possible. For more information, including important deadlines, please visit the Student Wellness website at:

<http://www.queensu.ca/studentwellness/accessibility-services/>

## **Copyright of Course Materials**

The following statement is pre-loaded into courses created on OnQ:

Course materials created by the course instructor, including all slides, presentations, handouts, tests, exams, and other similar course materials, are the intellectual property of the instructor. It is a departure from academic integrity to distribute, publicly post, sell or otherwise disseminate an instructor's course materials or to provide an instructor's course materials to anyone else for distribution, posting, sale or other means of dissemination, without the instructor's *express consent*. A student who engages in such conduct may be subject to penalty for a departure from academic integrity and may also face adverse legal consequences for infringement of intellectual property rights.

Please see Appendix B (page 8) for discussion of copyright options.

## **10. Privacy Statement for Instructors Who Use External Software in Their Course**

This course makes use of zoom for lectures and tutorials. Be aware that by logging into the site, you will be leaving onQ, and accessing zoom's website. Your independent use of that site, *beyond what is required for the course (for example, purchasing the company's products)*, is subject to zoom's terms of use and privacy policy. In addition, you are encouraged to review these documents, using the links below, before using the sites.

Links to the most common websites used by instructors are listed below:

- Crowdmark - <https://crowdmark.com/privacy/queens/>
- Pearson & Peer Scholar- <http://www.pearsoncanada.ca/pearson-canada-at-a-glance/legal/privacy-statement>
- Wiley - <https://www.wiley.com/en-ca/privacy>
- McGraw Hill - <https://www.mheducation.ca/privacy/>
- Turnitin - [http://turnitin.com/en\\_us/about-us/privacy](http://turnitin.com/en_us/about-us/privacy)
- Rosetta Stone (formerly Tell Me More) - [http://resources.rosetta-stone.com/CDN/us/agreements/US\\_Privacy\\_Policy-102513.pdf](http://resources.rosetta-stone.com/CDN/us/agreements/US_Privacy_Policy-102513.pdf)
- Coglab - <https://coglab.cengage.com/info/privacy.shtml>

### **Notice of Recording**

Synchronous (live) classes will be delivered in this course through a video conferencing platform supported by the University [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 I shall attempt to make them 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 me 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](#).

### **Accommodations for Disabilities**

Queen's University is committed to achieving full accessibility for people with disabilities. Part of this commitment includes arranging academic accommodations for students with disabilities to ensure they have an equitable opportunity to participate in all of their academic activities. The Senate Policy for Accommodations for Students with Disabilities was approved at Senate in November 2016 (see <https://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslclwww/files/files/policies/senate-andtrustees/ACADACCOMMPOLICY2016.pdf>). If you are a student with a disability and think you may need academic accommodations, you are strongly encouraged to contact the Queen's Student Accessibility Services (QSAS) and register as early as possible. For more information, including important deadlines, please visit the QSAS website at: <http://www.queensu.ca/studentwellness/accessibility-services/>

### **Academic Consideration for Students with 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.uslclwww/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. Please use the following:

Instructor/Coordinator Name: Tucker Carrington

Instructor/Coordinator email address: tucker.carrington@queensu.ca

## **15. 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.