

Quantum Mechanics CHEM/ENCH 313

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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, Hueckel method
- v) Molecules: the Born-Oppenheimer approximation
- vi) Time dependent problems: Absorption of radiation, inelastic scattering

Textbooks

Reference book: Quantum Chemistry, Donald A. McQuarrie, 2nd edition

Additional reading: Quantum Chemistry, Ira N. Levine, 7th edition

Both books are available in the library.

Marking Scheme

EVALUATION:

Midterm: 30%
Two assignments: 10%
Two quizzes: 10%
Final exam 50%

PROPOSED DATES:

First assignment due at the end of the lecture on the 20th of September

First Quiz 4th October

Midterm probably during the lecture on the 18th of October

Second assignment due the 1st of November

Second Quiz 15th November

Grading Method

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 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.**

For exams being offered remotely, Regulation 7.2.3. [Restrictions on Assessment](#) is waived.

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.

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.

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). 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.

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.”

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/>

Academic Considerations for Students in Extenuating Circumstances

The Senate Policy on Academic Consideration for Students in Extenuating Circumstances (<http://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslcwww/files/files/policies/senateandtrustees/Academic%20Considerations%20for%20Extenuating%20Circumstances%20Policy%20Final.pdf>) was approved in April, 2017. Queen's University is committed to providing academic consideration to students experiencing extenuating circumstances that are beyond their control and which have a direct and substantial impact on their ability to meet essential academic requirements. 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 they submit a request at: <http://www.queensu.ca/artsci/accommodations>.