Quantum Mechanics
CHEM/ENCH 313

Instructor: Tucker Carrington

Instructor Contact Information
Email: tucker.carrington@queensu.ca
Office: Chernoff Hall, Office 409
Office Hours: on request, any time. Send me an email to arrange a time.

TA: Sangeeth D. Kallullathil

TA Contact Information:
Email: sdk4@queensu.ca
Office: Chernoff Hall, Room 314

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
Both books are available in the library.

**Marking Scheme**

2 Assignments 10%
2 Quizzes 10%
Midterm 30%
Final exam (50%)

**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:

<table>
<thead>
<tr>
<th>Grade</th>
<th>Numerical Course Average (Range)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A+</td>
<td>90-100</td>
</tr>
<tr>
<td>A</td>
<td>85-89</td>
</tr>
<tr>
<td>A-</td>
<td>80-84</td>
</tr>
<tr>
<td>B+</td>
<td>77-79</td>
</tr>
<tr>
<td>B</td>
<td>73-76</td>
</tr>
<tr>
<td>B-</td>
<td>70-72</td>
</tr>
<tr>
<td>C+</td>
<td>67-69</td>
</tr>
<tr>
<td>C</td>
<td>63-66</td>
</tr>
<tr>
<td>C-</td>
<td>60-62</td>
</tr>
<tr>
<td>D+</td>
<td>57-59</td>
</tr>
<tr>
<td>D</td>
<td>53-56</td>
</tr>
<tr>
<td>D-</td>
<td>50-52</td>
</tr>
<tr>
<td>F</td>
<td>49 and below</td>
</tr>
</tbody>
</table>

**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 of the Location and Timing of Final Examinations**

As noted in Academic Regulation 8.2.1, “the final examination in any class offered in a term or session (including Summer Term) must be written on the campus on which it was taken, at the end of the appropriate term or session at the time scheduled by the Examinations Office.” The exam period is listed in the key dates prior to the start of the academic year in the Faculty of Arts and Science Academic Calendar and on the Office of the University Registrar’s webpage. A detailed exam schedule for the Fall Term is posted before the Thanksgiving holiday; for the Winter Term it is posted the Friday before Reading Week, and for the Summer Term the window of dates is noted on the Arts and Science Online syllabus prior to the start of the course. 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.

**Academic Integrity**

Queen’s students, faculty, administrators and staff all have responsibilities for supporting and upholding the fundamental values of academic integrity. Academic integrity is constituted by the five core fundamental values of honesty, trust, fairness, respect and responsibility (see www.academicintegrity.org) and by the quality of courage. These values and qualities 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. Students are responsible for familiarizing themselves with and adhering to the regulations concerning academic integrity. General information on academic integrity is available at Integrity@Queen's University, along with Faculty or School specific information. Departures from academic integrity include, but are not limited to, plagiarism, use of unauthorized materials, facilitation, forgery and falsification. Actions which contravene the regulation on academic integrity carry sanctions that can range from a warning, to loss of grades on an assignment, to failure of a course, to 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 only approved and permitted **calculator for Arts and Science courses and exams is the Cassio 991 series**. This calculator sells for around $25 at the Queen's Campus Bookstore, Staples and other popular suppliers of school and office supplies.

**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.