Introduction to Quantum Mechanics II  
Fall Semester 2019  
MWF, 9:35AM-10:40AM HEB 2002

Instructor: Rodrigo Noriega  
Email: noriega@chem.utah.edu  
Phone Number: (801) 579-7979  
Office Hours: By appointment. Please schedule meetings over email and at least 48hrs in advance.  
Office Location: TBBC 2428  
Preferred contact method: Email. If my office door is open, it means I’m available for drop-in consults.

Required Materials  
There is no required textbook, as there are many sources that cover the material in appropriate depth. For a list of books I find useful, see below (these are available at the University Library).  

Course Description  
An introduction to the electronic structure and symmetry of molecules, including point group theory, approximation methods and their limitations (the Born-Oppenheimer approximation, the Hartree-Fock SCF method, and several post-SCF methods). Use of quantum chemistry programs to calculate ground state molecular geometries, electronic wave functions, molecular orbitals, vibrational modes, and other molecular properties, including transition states for reaction. This course covers topics useful for chemists, physicists, and engineers, who have the necessary fundamental background in time-independent quantum mechanics

Pre-/co-requisites: Introduction to Quantum Mechanics I (CHEM 7000).  
Credit hours: 2.0

Course Outcomes  
By the end of this course, you will be able to:  
• employ symmetry constraints to solve Quantum Mechanical problems  
• extend the application of Quantum Mechanics to molecular systems  
• understand the Quantum-mechanical foundation of Computational Chemistry  
• be familiar with the formalism necessary to solve time-dependent Quantum-mechanical situations (e.g., spectroscopy)

Teaching and Learning Methods  
This course is primarily lecture-based. Lectures follow a discussion format, with a focus on core concepts and their implications. In-class discussion of homework is student-led. Exams and homework problems are geared to demonstrate the applicability of concepts from the course.
Supplemental Lectures
There will be 4 supplemental lectures (offered in the first half of Fall semester) that will cover mathematical concepts useful in Quantum Mechanics. A description of the goals, time, and location of these sessions can be found as an appendix to this syllabus.

University Policies

1. *The Americans with Disabilities Act.* The University of Utah seeks to provide equal access to its programs, services, and activities for people with disabilities. If you will need accommodations in this class, reasonable prior notice needs to be given to the Center for Disability Services, 162 Olpin Union Building, (801) 581-5020. CDS will work with you and the instructor to make arrangements for accommodations. All written information in this course can be made available in an alternative format with prior notification to the Center for Disability Services.

2. *University Safety Statement.* The University of Utah values the safety of all campus community members. To report suspicious activity or to request a courtesy escort, call campus police at 801-585-COPS (801-585-2677). You will receive important emergency alerts and safety messages regarding campus safety via text message. For more information regarding safety and to view available training resources, including helpful videos, visit [safeu.utah.edu](http://safeu.utah.edu).

3. *Addressing Sexual Misconduct.* Title IX makes it clear that violence and harassment based on sex and gender (which includes sexual orientation and gender identity/expression) is a civil rights offense subject to the same kinds of accountability and the same kinds of support applied to offenses against other protected categories such as race, national origin, color, religion, age, status as a person with a disability, veteran’s status, or genetic information. If you or someone you know has been harassed or assaulted, you are encouraged to report it to the Title IX Coordinator in the Office of Equal Opportunity and Affirmative Action, 135 Park Building, 801-581-8365, or the Office of the Dean of Students, 270 Union Building, 801-581-7066. For support and confidential consultation, contact the Center for Student Wellness, 426 SSB, 801-581-7776. To report to the police, contact the Department of Public Safety, 801-585-2677(COPS).

4. *Undocumented Student Support Statement.* Immigration is a complex phenomenon with broad impact—those who are directly affected by it, as well as those who are indirectly affected by their relationships with family members, friends, and loved ones. If your immigration status presents obstacles to engaging in specific activities or fulfilling specific course criteria, confidential arrangements may be requested from the Dream Center. Arrangements with the Dream Center will not jeopardize your student status, your financial aid, or any other part of your residence. The Dream Center offers a wide range of resources to support undocumented students (with and without DACA) as well as students from mixed-status families. To learn more, please contact the Dream Center at 801.213.3697 or visit [dream.utah.edu](http://dream.utah.edu).

5. *Drop/Withdrawal.* The last day to drop this course without paying tuition is Friday, October 18, 2019. After that date tuition is assessed. You may still withdraw from the course
according to the *University withdrawal policy*. Please check the academic calendar for more information pertaining to dropping and withdrawing from a course. Withdrawing from a course and other matters of registration are the student’s responsibility.

6. Other important information to consider including:
   a. Student Code: [http://regulations.utah.edu/academics/6-400.php](http://regulations.utah.edu/academics/6-400.php)
   b. Accommodation Policy (Section Q): [http://regulations.utah.edu/academics/6-100.php](http://regulations.utah.edu/academics/6-100.php)

7. **Wellness Statement.** Personal concerns such as stress, anxiety, relationship difficulties, depression, cross-cultural differences, etc., can interfere with a student’s ability to succeed and thrive and the University of Utah. For helpful resources, contact the Center for Student Wellness at [www.wellness.utah.edu](http://www.wellness.utah.edu) or (801) 581-7776.

8. **Veterans Center.** If you are a veteran, service member, or a family member of a current or former service member, the University of Utah has a variety of resources to help you receive the benefits you earned. Please visit the Veteran Services office ([https://registrar.utah.edu/veteran/](https://registrar.utah.edu/veteran/)) or the Veterans Support Center ([https://veteranscenter.utah.edu/](https://veteranscenter.utah.edu/)) for specific advice and guidance. Besides benefits concerns, they serve as a liaison between the student veteran community and the university, and they provide support to improve and enhance your individual and academic success.

9. **LGBT Resource Center.** If you are a member of the LGBTQ community, please be assured that this classroom is a safe zone. Additionally, the University of Utah has an LGBT Resource Center on campus (Room 409 in the Olpin Union Building, M-F 8am-5pm). You can visit their website to find more information about the support they can offer, a list of events through the center and links to additional resources at [http://lgbt.utah.edu/](http://lgbt.utah.edu/). Please also let the instructor know if there is any additional support you may need for this course.

10. **Learners of English as an Additional/Second Language.** If you are an English language learner, please be aware of several resources on campus that will support you with your language and writing development. These resources include:
    - The Writing Program – [http://writing-program.utah.edu/](http://writing-program.utah.edu/)
    - The English Language Institute – [http://continue.utah.edu/eli](http://continue.utah.edu/eli)
    Please let the instructors and/or TAs know if there is any additional support you would like to discuss for this class.

**Course Policies**

*Attendance & Punctuality:* Attendance to 100% of the lectures is not mandatory, yet highly recommended. Excessive absenteeism may result in penalties to your grade and may even result in failing the course. Please be on time for the lectures, as it is a relatively fast-paced course covering a substantial amount of material.

*Participation:* Participation in the discussion is encouraged and accounted for in your grade. To receive credit for class participation, you will need to lead the discussion of a homework problem during one of the assigned class sessions (volunteer or chosen at random).
**Food & Drink:** Food and drink in class or office hours are permitted as long as they are not disruptive or violate building/classroom regulations.

**Electronic Devices in Class:** Cell phones are not allowed in class. Laptops, notepads, etc. are OK if they serve an educational purpose (e.g., note-taking, follow lecture notes online).

**Canvas:** Canvas will be the main source for class material – lecture notes, homework assignments, exams will be posted there. Occasionally, announcements will be made.

**Assignments**
There will be 2 homework assignments, with 2-4 problems each. You can work on these homework assignments as a group, but every student is responsible for understanding every part of the solution and contribute to the discussion.
Exams will be take-home, individual, and with a 1-week time limit. You can use class notes when working on exams, but not textbooks, online solutions, etc. Computer-based solutions (e.g., integral solutions) are acceptable.

**Grading Policy**

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<thead>
<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Class participation/discussion</td>
<td>20%</td>
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<tr>
<td>Homework</td>
<td>20%</td>
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<tr>
<td>Midterm exam</td>
<td>20%</td>
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<tr>
<td>Final Exam</td>
<td>40%</td>
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*Note: This syllabus is meant to serve as an outline and guide for our course. Please note that I may modify it with reasonable notice to you. I may also modify the Course Schedule to accommodate the needs of our class. Any changes will be announced in class and posted on Canvas under Announcements.*
**Course Schedule**

All notes are available on Canvas and labeled by topics covered in them.

<table>
<thead>
<tr>
<th>Week 1:</th>
<th>Date</th>
<th>Topic/Discussion</th>
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<tbody>
<tr>
<td>Mon 10/14 - Fri 10/18</td>
<td>Symmetry and Group Theory</td>
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<tr>
<th>Week 2:</th>
<th>Date</th>
<th>Topic/Discussion</th>
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<tbody>
<tr>
<td>Mon 10/21 - Fri 10/25</td>
<td>Born-Oppenheimer approximation and its application</td>
<td>1^ST PROBLEM SET POSTED</td>
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<tr>
<th>Week 3:</th>
<th>Date</th>
<th>Topic/Discussion</th>
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<tbody>
<tr>
<td>Mon 10/28 - Fri 11/1</td>
<td>Molecular orbital theory introduction (homonuclear diatomics)</td>
<td>1^ST PROBLEM SET DUE</td>
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<tr>
<th>Week 4:</th>
<th>Date</th>
<th>Topic/Discussion</th>
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<tr>
<td>Mon 11/4 - Fri 11/8</td>
<td>Molecular orbital theory – heteronuclear diatomics and polyatomics</td>
<td>2^ND PROBLEM SET POSTED</td>
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<tr>
<th>Week 5:</th>
<th>Date</th>
<th>Topic/Discussion</th>
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<tr>
<td>Mon 11/11 - Fri 11/15</td>
<td>Computational chemistry (Hartree-Fock, Density Functional Theory)</td>
<td>2^ND PROBLEM SET DUE</td>
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**Week 6: | Date       | Topic/Discussion                                      |
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<tbody>
<tr>
<td>Mon 11/18 - Fri 11/22</td>
<td>Density matrix formalism, Feynman diagrams</td>
<td>MIDTERM EXAM DUE</td>
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<tr>
<th>Week 7:</th>
<th>Date</th>
<th>Topic/Discussion</th>
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<tbody>
<tr>
<td>Mon 11/25 - Fri 11/29</td>
<td>Time-dependent perturbation theory</td>
<td>MIDTERM EXAM DUE</td>
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Fri 11/29 is a University holiday (Thanksgiving)

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<th>Week 8:</th>
<th>Date</th>
<th>Topic/Discussion</th>
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<tbody>
<tr>
<td>Mon 12/2 - Wed 12/6</td>
<td>Review and Special Topics</td>
<td>FINAL EXAM POSTED</td>
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Last lecture is on Wed 12/4

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<th>Week 9:</th>
<th>Date</th>
<th>Topic/Discussion</th>
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<tbody>
<tr>
<td>Mon 12/9 - Fri 12/13</td>
<td>Finals Week</td>
<td>FINAL EXAM DUE</td>
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Final Exam due
APPENDIX

Math Concept Review – a sidekick to CHEM 7000 & 7010
Rodrigo Noriega
Department of Chemistry, University of Utah

Why? Quantum Mechanics (and Physical Chemistry in general) often use advanced Mathematics to develop abstract ideas. In order to provide students with the necessary tools to engage with the material presented in the Introduction to Quantum Mechanics course, I have put together the following short set of discussions. We will define mathematical concepts, practice their application, and discuss their use in Physical Chemistry and Quantum Mechanics.

When/where? These are optional, yet highly recommended, 2 hr sessions to be held at the start of the Fall semester. You do not need to be enrolled in CHEM 7000 to attend, so please share this with your fellow students if you think they’d be interested.

The location will be determined on the first day of class, once the day and time are set.

For students not currently taking CHEM 7000: I ask that you reach out to me first, as I need to reserve a room of the right size (email noriega@chem.utah.edu)

What?

Session 1
- Complex numbers
- Infinite series & Taylor expansion
- Limits and approximations
- Kronecker and Dirac delta functions

Session 2
- Coordinate systems
- Functional analysis (e.g., symmetry)
- Fourier transforms (or transforms in general)

Session 3
- Partial derivatives
- Differential equations
- Special functions (e.g., Legendre, Hermite, Bessel, Laguerre, spherical harmonics)

Session 4
- Linear algebra (e.g., eigenvalues, eigenstates, basis sets, Hilbert spaces)