

# Chemistry 544: Introduction to Quantum Chemistry

Fall 2017

**Instructor** Prof. Susumu Takahashi  
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**Lecture** Tue and Thu 9:00 – 10:20 am; SGM 307

**Discussion** Fri 11:00 - 11:50 am; SGM 226 (Exercises, discussions and makeup classes)

**Office Hours** Wed 1:00-2:00 pm and by appointment; LJS 152

## Course Description

This class provides an introduction to the basic principles of quantum mechanics and their applications to chemistry. A mathematics background substantially beyond proficiency in calculus (integration, differentiation, series), matrix representations, and linear algebra should not be necessary.

During the lectures, the postulates of quantum mechanics and operators and wave functions will be introduced. We will obtain stationary solutions for a variety of problems such as linear motion, the particle in a box problem, harmonic oscillator, 2-D and 3-D rigid rotor, and the hydrogen atom. We will also build non-stationary states and study their evolution in time. Group theory and perturbation theory will be introduced. Important mathematical techniques used in the problem will be reviewed in the lecture.

A part of the discussion session on Friday will be practical computer-based exercises using Matlab. No previous experience with Matlab is required. We will begin by writing programs for solutions to the problems mentioned above, and will use these solutions as bases for more complicated problems involving tunneling, a particle in an arbitrary potential, rotational-vibrational spectra of diatomic molecules, and spin-orbit coupling in the H atom. Students proficient with other computer applications such as Mathematica, can use them in class as well as for homework and projects, however such applications will not be supported by the instructor. Other parts of the discussion session will be used for reviews of the lectures and makeup classes.

**Textbook** Molecular Quantum Mechanics, Atkins and Friedman, 5<sup>th</sup> Edition (Chapters 1-7 will be covered).

**Website** <http://singlespin.usc.edu/teaching/index.html>

**Homework** Bi-weekly

**Exams** Midterm 1: 9-10 am, October 12th (Tentative).  
Midterm 2: 9-10 am, November 9th (Tentative)  
Final Exam: TBA

**Grade** Homework: 30%, Midterms: 40%, Final Exam: 30 %

**Academic Integrity**

USC seeks to maintain an optimal learning environment. General principles of academic honesty include the concept of respect for the intellectual property of others, the expectation that individual work will be submitted unless otherwise allowed by an instructor, and the obligations both to protect one's own academic work from misuse by others as well as to avoid using another's work as one's own. All students are expected to understand and abide by these principles. *SCampus*, the Student Guidebook, contains the Student Conduct Code in Section 11.00, while the recommended sanctions are located in Appendix A: <http://www.usc.edu/scampus/>. Students will be referred to the Office of Student Judicial Affairs and Community Standards for further review, should there be any suspicion of academic dishonesty. The review process can be found at: <http://www.usc.edu/student-affairs/SJACS/>.

**Holidays (No class)**

Thanksgiving: November 23th and 24th