

# Chemistry 544: Introduction to Quantum Chemistry

Fall 2023

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

**Office Hours** Wed: 1-2 pm in LJS 152 or on appointment

## 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.

Furthermore a part of the lectures 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.

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

**Homework** Bi-weekly

**Exams** Midterm 1: TBA  
Midterm 2: TBA  
Final Exam: 11-1 pm, December 7, Thursday

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

## Holidays (No class)

October 12 (Fall Recess) and November 23 (Thanksgiving)

## Statement on Academic Conduct and Support Systems

### Academic Conduct:

Plagiarism – presenting someone else’s ideas as your own, either verbatim or recast in your own words – is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in SCampus in Part B, Section 11, “Behavior Violating University Standards” [policy.usc.edu/scampus-part-b](https://policy.usc.edu/scampus-part-b). Other forms of academic dishonesty are equally unacceptable. See additional information in SCampus and university policies on scientific misconduct, [policy.usc.edu/scientific-misconduct](https://policy.usc.edu/scientific-misconduct).

### Support Systems:

*Counseling and Mental Health - (213) 740-9355 – 24/7 on call*

[studenthealth.usc.edu/counseling](https://studenthealth.usc.edu/counseling)

Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

*National Suicide Prevention Lifeline - 1 (800) 273-8255 – 24/7 on call*

[suicidepreventionlifeline.org](https://suicidepreventionlifeline.org)

Free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week.

*Relationship and Sexual Violence Prevention and Services (RSVP) - (213) 740-9355(WELL), press “0” after hours – 24/7 on call*

[studenthealth.usc.edu/sexual-assault](https://studenthealth.usc.edu/sexual-assault)

Free and confidential therapy services, workshops, and training for situations related to gender-based harm.

*Office of Equity and Diversity (OED)- (213) 740-5086 | Title IX – (213) 821-8298*

[equity.usc.edu](https://equity.usc.edu), [titleix.usc.edu](https://titleix.usc.edu)

Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants. The university prohibits discrimination or harassment based on the following *protected characteristics*: race, color, national origin, ancestry, religion, sex, gender, gender identity, gender expression, sexual orientation, age, physical disability, medical condition, mental disability, marital status, pregnancy, veteran status, genetic information, and any other characteristic which may be specified in applicable laws and governmental regulations. The university also prohibits sexual assault, non-consensual sexual contact, sexual misconduct, intimate partner violence, stalking, malicious dissuasion, retaliation, and violation of interim measures.

*Reporting Incidents of Bias or Harassment - (213) 740-5086 or (213) 821-8298*

[usc-advocate.symplicity.com/care\\_report](https://usc-advocate.symplicity.com/care_report)

Avenue to report incidents of bias, hate crimes, and microaggressions to the Office of Equity and Diversity |Title IX for appropriate investigation, supportive measures, and response.

*The Office of Disability Services and Programs - (213) 740-0776*

[dsp.usc.edu](https://dsp.usc.edu)

Support and accommodations for students with disabilities. Services include assistance in providing readers/notetakers/interpreters, special accommodations for test taking needs, assistance with architectural barriers, assistive technology, and support for individual needs.

ver. 2023/8/20

*Campus Support & Intervention - (213) 821-4710*

[campussupport.usc.edu](http://campussupport.usc.edu)

Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

*Diversity at USC - (213) 740-2101*

[diversity.usc.edu](http://diversity.usc.edu)

Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

*USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call*

[dps.usc.edu](http://dps.usc.edu), [emergency.usc.edu](http://emergency.usc.edu)

Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

*USC Department of Public Safety - UPC: (213) 740-6000, HSC: (323) 442-120 – 24/7 on call*

[dps.usc.edu](http://dps.usc.edu)

Non-emergency assistance or information.