

CHEM 645: Quantum Mechanics in Chemistry Spring 2017

CREDITS: 3

CLASS MEETING TIME: TTH, 11:00 AM -12:20 PM
LOCATION: 100 Life Science

INSTRUCTOR: Professor Ari Chakraborty
4-008 CST
ari.course@syr.edu

OFFICE HOURS: Held in room CST 0-10
Thursday 1-2 pm
and by appointment.

COURSE MANAGEMENT SYSTEM: <http://blackboard.syr.edu/>

The site will have class information posted including:

- Lecture notes
- Test schedules, results, and post-exam answers
- Homework assignments
- Other important class information

RECOMMENDED BOOKS:

[1]. [Quantum Mechanics by R. Shankar](#)

[2]. [Modern Quantum Chemistry: Introduction to advanced electronic structure theory by Attila Szabo and Neil S. Ostlund \(Dover Publications\)](#)

[3]. [Density functional theory of atoms and molecules by Parr and Yang \(Ebook available from SU library\)](#)

DESCRIPTION:

Application of quantum mechanics in chemistry with emphasis on electronic structure theory, chemical dynamics, and spectroscopy.

Topics covered:

- Review of complex numbers, linear algebra, and vector spaces
- Representation theory (Dirac, Schrödinger, Heisenberg)
- Postulates of quantum mechanics
- Commutator algebra
- Position and momentum basis representation
- Time-dependent and time-independent Schrödinger equation
- Exactly solvable models
- Approximate methods for solving time-independent systems
- Many-particle systems and electron correlation
- Survey of various quantum chemical methods: Hartree-Fock, perturbation theory, configuration interaction, coupled-cluster, quantum Monte Carlo, density-matrix theory
- Introduction of density functional theory: key theorems and results

PREREQUISITES:

If you have any questions about your preparation for this course, you should talk to the instructor as soon as possible.

Students with any type of disability who may need special consideration or accommodations are encouraged to discuss their concerns with the instructor right away to make arrangements.

More information on <http://supolicies.syr.edu/>

EVALUATION:

Final Exam:	40%
Homework Assignments:	30%
Quizzes:	30%

COURSE POLICIES

Academic Honesty (from <http://academicintegrity.syr.edu>)

Syracuse University's Academic Integrity Policy reflects the high value that we, as a university community, place on honesty in academic work. The policy defines our expectations for academic honesty and holds students accountable for the integrity of all work they submit. Students should understand that it is their responsibility to learn about course-specific expectations, as well as about university-wide academic integrity expectations. The policy governs appropriate citation and use of sources, the integrity of work submitted in exams and assignments, and the veracity of signatures on attendance sheets and other verification of participation in class activities. The policy also prohibits students from submitting the same work in more than one class without receiving written authorization in advance from both instructors. Under the policy, students found in violation are subject to grade sanctions determined by the course instructor and non-grade sanctions determined by the School or College where the course is offered as described in the Violation and Sanction Classification Rubric. SU students are required to read an online summary of the University's academic integrity expectations and provide an electronic signature agreeing to abide by them twice a year during pre-term check-in on MySlice. For more information about the policy, see <http://academicintegrity.syr.edu>.

The Violation and Sanction Classification Rubric establishes recommended guidelines for the determination of grade penalties by faculty and instructors, while also giving them discretion to select the grade penalty they believe most suitable, including course failure, regardless of violation level. Any established violation in this course may result in course failure regardless of violation level.

Attendance

Attendance is not recorded in lecture. However, there is a very strong correlation with good attendance and good grades and it is in your own best interest to attend lectures regularly.

Syracuse University's religious observances policy

(http://supolicies.syr.edu/emp_ben/religious_observance.htm) recognizes the diversity of faiths represented among the campus community and protects the rights of students, faculty, and staff to observe religious holy days according to their tradition. Under the policy, students are

provided an opportunity to make up any examination, study, or work requirements that may be missed due to a religious observance provided they notify their instructors before the end of the second week of classes. For fall and spring semesters, an online notification process is available through MySlice/Student Services/Enrollment/My Religious Observances from the first day of class until the end of the second week of class. The religious observances policy requires accommodation for the religious holiday itself, not for travel days if a student will be observing the holiday elsewhere.

Medical absences will be excused based on written advice from the Health Center or a health-care provider (based upon clinical findings and prescribed treatment recommendations). **NO VERBAL EXCUSES WILL BE ACCEPTED.** The medical document must specifically indicate that you were unable to attend class/recitation. All such absences will be verified by Chemistry Department staff.

THERE WILL BE NO MAKEUP EXAMINATIONS EXCEPT IN THE CASE OF ADVANCE-NOTICE APPROVED ABSENCES.

ALL ADVANCED-NOTICE APPROVALS WILL RESULT IN AN OPPORTUNITY TO TAKE THE EXAM IN ADVANCE, NOT AFTER THE REGULARLY SCHEDULED EXAM TIME.

AN APPROVED ABSENCE THAT PREVENTS A STUDENT FROM TAKING AN EXAM ON-TIME OR EARLY WILL RESULT IN THE DROPPING OF THAT PARTICULAR GRADE FROM THE CALCULATION OF THE OVERALL CLASS GRADE.

Disability-Related Issues

If you have a learning or physical disability, please see Professor Chakraborty as soon as possible (**during the first 2 weeks of the course**) to arrange for appropriate accommodations. No provisions/accommodations will be made if the instructor is notified after examinations. Students requiring special accommodations **MUST** register with the Office of Disability Services (804 University Avenue Room 309, Phone: Voice: (315) 443-4498; TDD: (315) 443-1371, E-Mail: odssched@syr.edu). Exams **MUST** be administered by the Office of Disability Services.

ACADEMIC ETHICS:

Possession of unauthorized materials during exams, alteration of exams prior to submission for regrading, plagiarism, or other forms of cheating will be considered serious violations of academic ethics and treated as such. They may result in a failing grade on an exam or in the course and may also be referred to the University disciplinary system.

All Syracuse University policies (<http://supolicies.syr.edu/>) regarding ethics and honorable behavior apply to this course.