Quantum Chemistry
Course Syllabus – Fall 2022

Courses: **CHEM 4120**, **CHEM 4120 HON**, and **CHEM 6120**
Instructor: Samer Gozem
E-mail: sgozem@gsu.edu

Office Hours: Please email me (sgozem@gsu.edu) if you would like to set up a time to meet in person or virtually.

Teaching Assistant: Sarah Ake
E-mail: sake1@student.gsu.edu

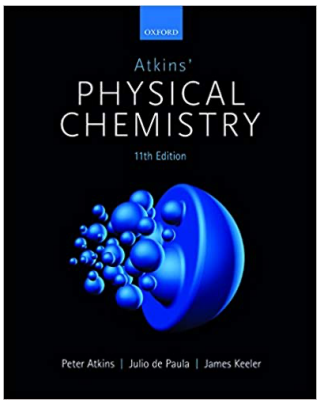
Instruction Mode: Face-to-face. Lectures TR, 3:45-5:00 pm in PSC 171.

Course Prerequisites: This course relies heavily on chemistry, physics, and math concepts from CHEM 1212K, PHYS 2212K, and MATH 2202 or 2212.

Course overview: The course has six modules, each lasting around 2-3 weeks.

Textbook: "**Physical Chemistry**" by Peter Atkins, Julio de Paula, and James Keeler, 11th Edition, Oxford University Press, 2017, ISBN 9780198769866. A few notes and tips:

- It is possible to complete the course without having the textbook. However, this is an excellent resource that explains all the topics from the class, often in a way that complements the lectures rather than just mirrors it.
- The textbook is available from several resources online, both as a rental and to buy.
- An older edition of the same textbook is fine.
- The full Atkins book has ~900 pages and has a black and blue cover. However, the publishers also have released the same book in three volumes. Most of the material in this course is from volume 2. Please be sure to get either the full textbook or volume 2 (volume 2 has the same cover but in orange instead of a blue image).
- If you plan to take Chem 4110 soon, you may need the Atkins book again. In that case, it might be a good idea to invest in the full book and/or rent for longer.



Student Resources: Resources accompanying the Atkins textbook, including additional information and the student solutions manual, are available at https://oup-arc.com/access/pchem11e-student-resources#tag_a-deeper-look.

Course Description: "Quantum Chemistry" is a 3-credit semester course that covers the principles atomic and molecular structure (quantum chemistry) and statistical mechanics. These topics serve as the basis for understanding molecular and spectroscopic properties. Focuses 7-11 and 13 from the textbook will be covered in this course.

Course Objectives: The overall objective is to understand the behavior of matter by deriving their properties at the atomic or molecular level from first principles. Students will also learn how to connect this molecular-level understanding with bulk properties through statistical mechanics.

Homework, Extra Problems, and No-credit Practice Problems: For each module, everyone will be assigned required homework. Homework will be available on iCollege at the start of each module and will typically be due the following Friday (10 days later, don't forget to submit before the deadline!). Homework can be attempted as many times as you like to fix wrong answers, but students must re-answer all questions in each attempt. Note that some questions on the exams will be very similar in format to homework questions. Mastering homework will go a long way towards better performance on exams. Chem 4120 HON and Chem 6120 students will also be assigned additional problems due on the same day. Finally, optional no-credit problems from the textbook will be recommended for everyone wanting extra practice.

Exams: There will be six exams in this course, one for each module. The lowest exam score will be dropped and replaced by the average of the other five exams. These exams will not be given at any time other than the scheduled lecture period (see make-up policy below). Each exam will primarily test your knowledge of the corresponding module. However, some of the questions on each exam may come from previous modules. There will be no other midterm or final exam.

Exam policies:

- The exams will be open book. You may use the book, your notes, and your calculator during exams. Please consider that you will not have a lot of time to browse through your book/notes, so use your time wisely.
- Cell phones must be turned OFF (not just silent) during all exams. Cell phones must not be in any place that is visible to you or me during the exam. In case of an emergency where you anticipate you might need your phone turned on during your exam, you must clear that with me first. You cell phones may **not** be used in place of a calculator for the exams.
- I reserve the right to move anyone during exams without explanation. I typically use this simply to spread people out. If you are asked to relocate, please collect your exam and notes and move to the newly assigned seat as quietly as possible.

Exam make-up policies:

- At the end of the semester, there will be one make-up exam available that can be taken by anyone who has missed an exam during the semester. This exam will be comprehensive. The difficulty of the exam will be like the other exams.
- Note that if you miss one exam, you also simply have the option to use it as your drop grade and not take the make-up exam. In this case, the exam will be assigned a grade equal to the average of the other five exams.
- If you miss two exams during the semester, you can make up one and use the other as the drop grade.
- Any additional exams missed will be assigned a grade of zero.
- When multiple missed exams and/or assignments are due to ongoing illness or hardship during this semester, please talk with your instructor as soon as you can to discuss early withdrawal, emergency withdrawal, or incomplete grade options. Incompletes are only assigned if students have completed most of the required material for the course and have a passing grade at the "last day to withdraw" date.

Discussion Forums: For each module, there will be two discussion forums:

- One forum is for questions and answers. Questions about lectures, homework, and additional practice problems can be discussed here. All students can either post questions or reply to questions. However, please do not give direct answers to homework questions.
- The second forum is for resources. Feel free to post any relevant reading material, videos, websites, or notes you found useful.

Participation: Participation will primarily be assessed based on contributions to the discussion forum (although, active participation during lectures may eliminate the need for online discussion). Simply:
No participation = no point.
Minimal participation (e.g., reading forum posts but not contributing) = partial points.
Actively posting to the discussion forums or regularly participating in lecture Q&As = full points.

Grading:
The grade breakdown for this course is as follows:

Module	%
1	16
2	16
3	16
4	16
5	20
6	16
Total	100

Here is the breakdown of grades for each module

	Chem 4120 (%)	Chem 4120HON/6120 (%)
Participation	5	5
Homework	45	30
Exam	50	50
Extra problems	0 (not required)	15

The following plus/minus grading system will be used for everyone:

Grade	**%**
A+	98+
A	90-98
A-	87-90
B+	84-87
B	80-84
B-	75-80
C+	70-75
C	65-70
C-	60-65
D	50-60
F	< 50

Last day to withdraw is **Tuesday, October 11th, 2022**
The University requires faculty, on a date set by the provost after the mid-point of the course,
1. to give a WF to all those students who are on their rolls but no longer taking the class, and
2. to report the last day the student attended or turned in an assignment.

Student Integrity Policy: All exams and assignments must represent the student's individual, unaided efforts. Receiving unauthorized outside information or offering unauthorized information to another student during an examinations or assignments is cheating. This includes the use of online "tutoring" or "study" tools while solving assignments, such as Chegg, which counts as unauthorized help. Any suspected offenses will be referred to the Department of Chemistry and the College of Arts and Sciences for appropriate action. Please refer to GSU's Academic Honesty Policy for more information.

Accommodations: Students who wish to request accommodation for a disability may do so by registering with the Access and Accommodation Center. Students may only be accommodated upon issuance by the Access and Accommodation Center of a signed **Accommodation Plan** and are responsible for providing a copy of that plan to instructors of all classes in which accommodations are sought.

Family Educational Rights and Privacy Act: In keeping with USG and university policy, this course website will make every effort to maintain the privacy and accuracy of your personal information. Specifically, unless otherwise noted, it will not actively share personal information gathered from the site with anyone except university employees whose responsibilities require access to said records. However, some information collected from the site may be subject to the Georgia Open Records Act. This means that while we do not actively share information, in some cases we may be compelled by law to release information gathered from the site. Also, the site will be managed in compliance with the Family Educational Rights and Privacy Act (FERPA), which prohibits the release of education records without student permission. For more details on FERPA, go here.

Course Evaluation: Your constructive assessment of this course plays an indispensable role in shaping education at Georgia State. Upon completing the course, please take time to fill out the online course evaluation.

Modules and course schedule:

The course syllabus provides a general plan for the course; please note that deviations may be necessary.

If you miss the deadline for homework or can't attend exams for reasons outside of your control (i.e., emergencies) please notify me as soon as you could.
Holidays: Labor Day: Monday, Sept 5. Thanksgiving Break: Nov 21-Nov 25.

Module	Chapters in book	Start date	HW Due date	Exam Date	% of final grade
1	Topics 7a-c	8/23	9/9	9/13	16
2	Topics 7d-e	9/13	9/23	9/27	16
3	Focus 8	9/27	10/7	10/11	16
4	Focus 9	10/11	10/21	10/25	16
5	Focus 11	10/25	11/11	11/15	20
6	Focus 13	11/15	12/2	12/6*	16

*Exam time on 12/6: 2:00 pm.

The following pages will list specific learning outcomes and tasks for each module.

Module 1 (M1): Introduction to Quantum Chemistry

Outcomes:

- Identify different subfields of physical chemistry and their relationship.
- Define some basic but important terms that will be used throughout this course.
- Review some of the major scientific problems that could not be solved by classical mechanics.
- Discuss the nature of light
- Discuss the nature of other particles.
- Define a wavefunction and the Born interpretation of a wavefunction.
- Construct eigenvalue equations with different operators and discuss their properties.
- Explain the uncertainty principle.
- Explain the postulates of quantum mechanics.

Tasks:

1. Attend M1 lectures.
2. Familiarize yourself with the syllabus.
3. Read Topics 7A-7C in the textbook.
4. Post questions, answers, comments, or resources in the M1 discussion forum.
5. Complete the M1 homework and submit by due date.
6. Take the M1 exam.

Module 2 (M2): Solving the Schrödinger equation with different potentials.

Outcomes:

- Apply quantum mechanics to translational motion.
- Use the particle in a box model to discuss degeneracy and quantum tunnelling.
- Apply quantum mechanics to vibrational motion.
- Apply quantum mechanics to rotational motion and define angular momentum.

Tasks:

1. Attend M2 lectures.
2. Read Topics 7D-7F in the textbook.
3. Post questions, answers, comments, or resources in the M2 discussion forum.
4. Complete the M2 homework and submit by due date.
5. Take the M2 exam.

Module 3 (M3): Atomic Structure and Spectra.

Outcomes:

- Apply quantum mechanics to the hydrogen and hydrogen-like atoms.
- Use the hydrogen atom solution to the Shdroginer equation to discuss the electronic structure of hydrogen.
- Extend the lessons from hydrogen to many-electron atoms.
- Explain the Pauli exclusion principle and use.
- Determine the electronic configurations of many-electron atoms.
- Use the rules of quantum mechanics to discuss the spectra of hydrogen and many-electron atoms.
- Define spin-orbit coupling.

Tasks:

1. Attend M3 lectures.
2. Read Focus 8 in the textbook.
3. Post questions, answers, comments, or resources in the M3 discussion forum.
4. Complete the M3 homework and submit by due date.
5. Take the M3 Exam.

Module 4 (M4): Molecular structure.

Outcomes:

- Apply valence-bond theory to explain molecular bonding.
- Apply molecular orbital theory to explain molecular bonding in different diatomic and polyatomic molecules.
- Define photoelectron spectroscopy and how it relates to molecular electronic structure.
- Discuss the variational principle and its application in molecular orbital theory.
- Discuss the Huckel approximation and other approximate solutions for solving electronic structure of polyatomic molecules.

Tasks:

1. Attend M4 lectures.
2. Read Focus 9 in the textbook.
3. Post questions, answers, comments, or resources in the M4 discussion forum.
4. Complete the M4 homework and submit by due date.
5. Take the M4 Exam.

Module 5 (M5): Molecular symmetry and spectroscopy.

Note: this is a three-week module.

Outcomes:

- (Time permitting) learn how molecular symmetry can determine molecular properties.
- (Time permitting) apply group theory to problems in molecular spectroscopy.
- Discuss electronic transitions in molecules and associated properties and experimental techniques.
- Discuss spectroscopies that probe rotational motion in molecules.
- Discuss spectroscopies that probe vibrational motion in molecules
- Explain how vibrtonic features arise in electronic transitions and excited-state decay.

Tasks:

1. Attend M5 lectures.
2. Read Topics 11A-11D in the textbook. We may also cover Focus 10 and/or topics 11F-11G, time-permitting.
3. Post questions, answers, comments, or resources in the M5 discussion forum.
4. Complete the M5 homework and submit by due date.
5. Take the M5 exam.

Module 6 (M6): Statistical Mechanics.

Outcomes:

- Introduce and discuss the Boltzmann distribution and molecular partition functions.
- Determine mean molecular energies from the partition function.
- Determine the relation between partition functions and internal energy, heat capacity, statistical entropy, and residual entropy.
- Derive thermodynamic functions (e.g., free energies) from the canonical partition function.
- Define equilibria from a statistical mechanics perspective.

Tasks:

1. Attend M6 lectures.
2. Read Focus 13 the textbook.
3. Post questions, answers, comments, or resources in the M6 discussion forum.
4. Complete the M6 homework and submit by due date.
5. Take the M6 exam.