1 ‖ General Information

- Class information: MWF 9:00–9:50 am, TLC 3210
- Final exam due: Thursday, March 21, 11:59 pm
- Recommended textbook: Physical Chemistry: A Molecular Approach (McQuarrie & Simon)
- Office hours (KNC): See Canvas
- TA: Adam Culick (aaculick@ucdavis.edu), see Canvas for office hours
  - Section A01 Discussion: M 6:10–7:00 pm, Wellman 127
  - Section A02 Discussion: T 8:00–8:50 am, Robbins 146

2 ‖ Course overview

This course covers quantum mechanics as applied to molecules, as well as an introduction to molecular spectroscopy and statistical thermodynamics. We will begin by examining the nature of the electronic wavefunction in polyatomic molecules and the computational approximations commonly used to solve the Schrödinger equation for molecular systems. We will then discuss the ways in which symmetry can be used to simplify quantum mechanical calculations on molecular systems, identify important types of intramolecular interactions, and rapidly give qualitative information about the properties of the molecular wavefunction. In the spectroscopy section, we will see how eigenstates of the molecular Hamiltonian can be interrogated using electromagnetic radiation. And finally, we will examine properties and distributions that arise from ensembles of molecular quantum systems.

On the whole, the objective of this course is to expose you to the physical foundations governing the behavior of molecules, to see how the energy levels predicted by quantum mechanics can be observed and how they affect bulk properties. While mathematics and calculations will certainly be a significant component of the course, the more important aspect will be understanding the conceptual underpinnings of the material. It is my philosophy that the course assignments should complement and extend the material covered in the course, not simply repeat simple calculations; furthermore, the exams will require you to apply the physical concepts we cover in new ways that you may not have previously seen. For these reasons, I strongly encourage you to join a study group on this course to help each other learn the key concepts. Please see below how the grading system in this course is structured to reward collaboration.

By the end of this course, you should be able to:

- Explain molecular bonding and geometry in terms of molecular orbital theory.
- Identify the point group of a molecule by examining its symmetry elements.
- Use a character table to decompose a reducible representation into its irreducible components.
- Analyze spectroscopic features of molecules.
- Explain how intermolecular forces affect the properties of bulk gases.
- Calculate partition functions and use partition functions to evaluate bulk thermodynamic properties.
- Determine distributions of molecular ensembles among quantum states.
- Explain the principles of lasers and their use in spectroscopy (time permitting).

3 ‖ Grading

I anticipate that this class will be graded on a curve based on the weighted total scores (see table below for the weights of each category). The curve will only be used to raise grades; for instance, a total weighted score of 79% is guaranteed to be a C+ or better. The mean of the curve will be initially set to 80% (B−), but the mean may be raised depending on the class performance on the midterms and final exam.

Item	Weight (%)
Pre-lecture quizzes	10
Discussion participation	10
Midterm exams	40 (2 × 20)
Final exam	40

Pre-lecture "Quizzes" Before most lectures, I will distribute a short, quick quiz the previous day (details via Canvas); it will cover material from both the previous and the upcoming class. These questions should take no more than 5–10 minutes to answer, and are intended to help you identify key points and practice applying course concepts. You will receive credit for completing each question on the quiz regardless of whether your answers are correct. While the number of points on each quiz may vary; each will count equally toward your course grade.

Discussion Participation Participation in weekly discussion sections is required. At each discussion session, a short one-question quiz similar to a pre-lecture quiz question will be given. Like pre-lecture quizzes, full credit will be awarded for completing the quiz regardless of whether the answers are correct.

Problem sets Optional weekly problem sets will be assigned and are due on the dates specified on the schedule below. All work will be submitted on Canvas by 11:59 pm on the indicated date. Late homework will be penalized by 50%. A detailed answer key will be posted at the end of the following class, **and late homework will not be accepted after this time.** Although optional, these problem sets will be graded and your score used to calculate a bonus that will be applied to your next exam according to the formula:

$$\text{Bonus\%} = \text{Min}\left(\frac{\text{HW\%} \times (150 - 15\sqrt{\text{Exam\%}})}{180}, \quad 0.3 \times \text{HW\%}\right).$$

The bonus is capped at 30% of your homework score. See the end of the syllabus for graphs illustrating the effect of the bonus.

Exams Both midterms and the final will be take-home exams (see below for the schedule). The first midterm will cover the course material on electronic structure, computational chemistry, and group theory, and the second will cover spectroscopy. No problem set will be due on the week of an exam, and there will be no class on the day an exam is due. The final exam covers the course as a whole but is weighted a bit more toward the material presented at the end of the course.

Additional notes on exams:

Timing: Exams will be posted to Canvas at least 24 hours before they are due, and on that day there will be no lecture. The exams are open-book, open-notes, and you may search for information online. You may not, however, communicate with anyone about the exam. This includes using online services like Chegg or other forums where you can post questions for others to answer.

Score replacement: If your final exam score is higher than your lowest midterm score, I will replace that midterm with your final exam score.

Course mean: As mentioned above, the course mean can be affected by the class's performance on the exams. The decision will be based on the raw exam scores. I encourage you to study together to help everyone understand the material.

4 ‖ Academic Integrity

You are expected to abide by the University's Code of Academic Conduct. If you are unsure about any point of academic ethics, or if you are concerned about potential unethical behavior, please do not hesitate to contact me or Student Judicial Affairs. Specific points related to this course:

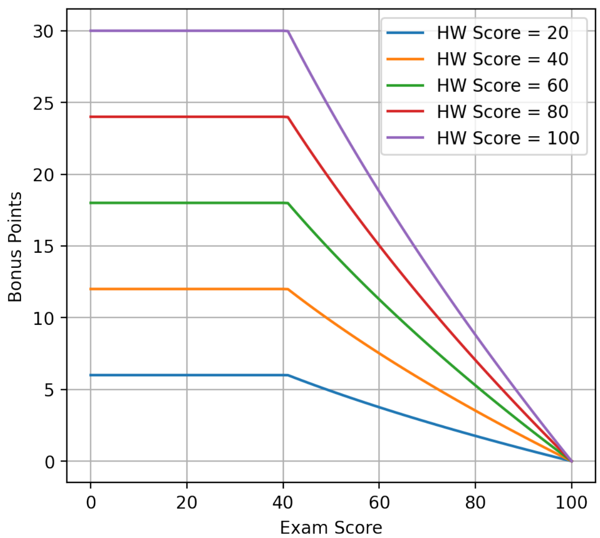
- Collaboration on problem sets is encouraged, but do not simply copy another student's work.
- Using answer keys from previous versions of this course to assist with problem sets is not allowed. Suspected instances of copying or paraphrasing past answer keys will be referred to Student Judicial Affairs. If SJA concludes that cheating took place, **bonus points will be forfeited on all exams**.
- The exams in this course are intended for you to work on independently. You may not communicate with anyone else about the problems on the exams, and under no circumstances are you to use answers given to you by another person, whether in the class or though use of any online Q&A services. **Suspected instances of collaboration or other cheating on exams will be reported to Student Judicial Affairs.** This could result in receiving 0 points for the exam in question.

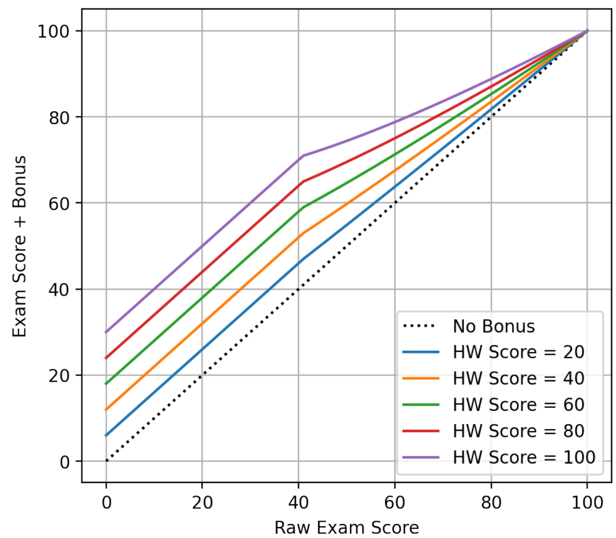
5 ‖ Tentative Schedule

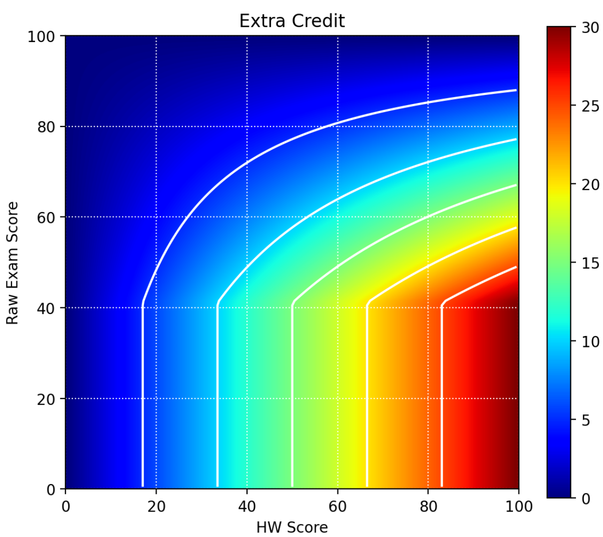
Week	Monday	Wednesday	Friday
1.8–1.12	Electronic structure	Electronic structure	Electronic structure
1.15–1.19	**MLK Jr Day**	Computational chemistry **PS 1 due**	Computational chemistry
1.22–1.25	Computational chemistry	Group theory **PS 2 due**	Group theory
1.29–2.2	Group theory	Group theory MT 1 cutoff **PS3 Due**	Spectroscopy
2.5–2.9	Spectroscopy	**MT 1 due**	Spectroscopy
2.12–2.16	Spectroscopy	Spectroscopy **PS 4 due**	Spectroscopy
2.19–2.23	**Presidents Day**	Spectroscopy **PS 5 due**	Spectroscopy
2.26–3.1	Spectroscopy MT 2 Cutoff	Gases & intermolecular forces	**MT 2 due**
3.4–3.8	Gases & intermolecular forces	Statistical thermodynamics	Statistical thermodynamics **PS 6 due**
3.12 – 3.15	Statistical thermodynamics	Statistical thermodynamics	Statistical thermodynamics **PS 7 due**
3.18–3.22	**Thursday, 3.21: Final exam due**		

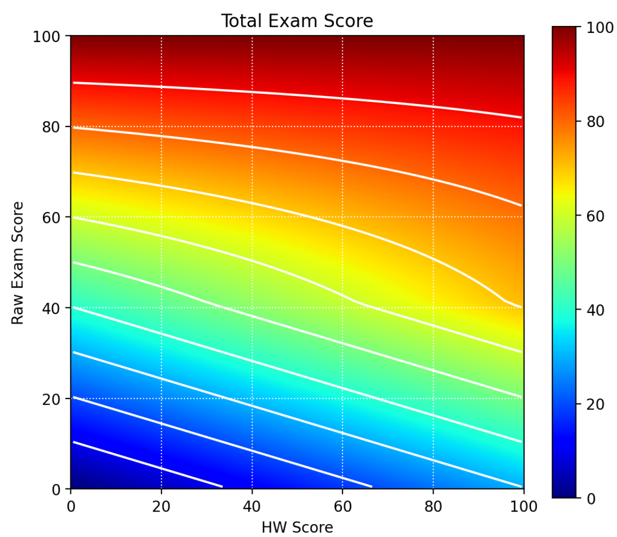
6 ‖ Exam Bonus

In order to help students who struggle with exams, bonus points are awarded for completing the optional weekly problems sets. Bonus points awarded are based on both your problem set score and your exam score: the higher the exam score, the lower the bonus. The first figure on the next page shows the number of bonus points as a function of exam score, and the second figure shows that the total exam score (with bonus included) increases monotonically. There is no advantage in scoring lower on the exams, but if you do score lower, then your homework performance will count for more of your grade. The bonus for midterm 1 is based on PS 1-3, for midterm 2: PS 4-5, and for the final: PS 6-7.


HW Score = 20
HW Score = 40
HW Score = 60
HW Score = 80
HW Score = 100
Bonus Points
Exam Score
0
5
10
15
20
25
30
0
20
40
60
80
100


No Bonus
HW Score = 20
HW Score = 40
HW Score = 60
HW Score = 80
HW Score = 100
Exam Score + Bonus
Raw Exam Score
0
20
40
60
80
100


Extra Credit
Raw Exam Score
HW Score
0
20
40
60
80
100
0
5
10
15
20
25
30


Total Exam Score
Raw Exam Score
HW Score
0
20
40
60
80
100