

# SYLLABUS

*CHEMISTRY 5591 – ADVANCED MOLECULAR SPECTROSCOPY*

*SPRING 2021, 3 CREDIT HOURS*

## INSTRUCTOR INFORMATION

Name: J. Mathias Weber

My office hours are tentatively on Wednesdays 4 – 5 pm and Thursdays 5 – 6 pm, and by appointment. The times and days of the office hours may shift during the semester to allow everyone in this course to make it to at least one office hour per week. This syllabus will be updated accordingly.

You can reach me at [weberjm@jila.colorado.edu](mailto:weberjm@jila.colorado.edu).

The office hours will take place via Zoom at <https://cuboulder.zoom.us/j/98490583428>.

## COURSE INFORMATION

**Formal course prerequisites:** Two semesters of physical chemistry and graduate standing, or instructor consent.

**Recommended:** Firm grasp of algebra, complex numbers, calculus, and differential equations, CHEM 5581 (Introductory Quantum Chemistry) or physics graduate course in quantum mechanics.

### **Course description and purpose:**

In this course, the basic principles of interaction of light and matter and their application in spectroscopy of atoms and molecules will be covered. You will learn how to describe absorption and emission of light by atoms and molecules, and how to characterize atomic and molecular states and molecular behavior by spectroscopy.

### **Lectures:**

Much of the course material will be covered in lectures. Please do not come late to class, because this disrupts the attention of your classmates. The lectures are a critical component of this course, and you are expected to attend. Students who attend classes perform on average much higher than those who do not (who would have thought that ...). Your participation in class both in asking and discussing relevant questions will be welcomed.

**Clickers:**

To facilitate your engagement (which will increase your learning success), and to provide feedback to you and me about where you are in your thinking, we will use the iClicker Reef system in class. Each student must have an iClicker Reef account to participate in clicker questions presented in lecture. The number of clicker questions will vary, but you should expect questions each class period. Clicker questions are presented in multiple-choice format. Depending on the purpose for asking a particular question, you may be asked to answer on your own or to discuss possible reasoning with students around you. Sometimes you may be asked a question about a topic you haven't yet encountered in class; at other times, you'll be asked to apply what you have just learned. In any case, it's important that you answer honestly as this provides the most accurate assessment of the class's thinking to me, and what comes next in lecture may depend on how the class responds. You should always be prepared to discuss your reasoning for your answer.

Please register set up your iClicker Reef account at:

<https://oit.colorado.edu/tutorial/cuclickers-set-iclicker-reef-student-account>

**Office Hours:**

Office hours will be on Wednesdays 4 – 5 pm and Thursdays 5 – 6 pm. These office hours are thought as an opportunity for you to ask any questions to clarify your understanding of the material. Always remember that there is no such thing as a dumb question! Please use the office hours, not email, for questions. If you email questions, I will only be able to answer them if I have time to do so during the office hours. If you cannot make the scheduled office hours in a given week, I will try to arrange an alternative time for you. If you come to me for help with homework, I expect that you have already tried to solve the problems yourself for a few hours.

## TEXTBOOKS AND MATERIALS

- Wolfgang Demtröder “Molecular Physics”. This is to some extent the main text book for the course. The lectures do not strictly follow the book, but most of the content of the lectures can be found there.
- Wolfgang Demtröder “Laser Spectroscopy”. This book contains many helpful concepts of spectroscopy techniques and lasers.
- I encourage you to look for other texts that you like. You can discuss them with me.

## ASSIGNMENTS

Homework assignments (problem sets and reading assignments) are an important part of the course as they should enhance your understanding of the material. You will have to use computer programs to generate function graphs, calculations, etc. for some of the homework assignments. Unless otherwise noted, you may use the programs of your choice to do this, provided you can achieve the objective with them.

The homework for this class will contain a number of problems where you will be asked to use a mathematically oriented programming language. The aim is to get you acquainted with simple programming if you are not already proficient in such a language, and to keep you using this skill if you already have some proficiencies in this area. The software package or programming language you will use will be completely up to you. You could use, e.g., Python, Matlab, Mathematica. If you already have experience with a certain language, you are of course welcome to use it. For the most part, I will post sample solutions based on Python, but that should not deter you from using a different language that you feel more comfortable with. Also, you don't need to expect that you will have to do involved coding. These problems and exercises are just meant to let you explore simple programming exercises in the context of spectroscopy. Some of you may view these problems as too trivial compared with your expectations and existing skills, and I will welcome feedback on this issue.

Assignments will usually be posted on Fridays on the course web site in Canvas. They are usually to be returned the following Fridays before class, but the due dates will be listed on each assignment. Unless otherwise specified, homework assignments must be returned as a single pdf file through the Canvas page. They can be handwritten (except where computer-generated material is required) and then scanned or photographed, or they can also be typed.

In addition to homework assignments you are expected to read the relevant textbook chapters and sometimes additional material.

## EXAMS

There will be two two-hour-exams and a final exam. It may be that at least one of the exams is a take-home exam, but currently they are scheduled as follows:

Scheduled dates for two-hour exams:

Exam 1: Tuesday, March 2, 2021, 6 p.m.–8 p.m., via Zoom

Exam 2: Tuesday, April 6, 2021, 6 p.m.–8 p.m., via Zoom

If there are problems with these exam dates, you must indicate these conflicts before Friday, January 29, 2021! There will be no makeup exams. The grade on an excused exam will be replaced by your average of the other exams, scaled by the class average on the missed exam. Exams missed without valid excuse will count as an F.

Final exam: Time and location will be announced at a later date.

## EXTRA CREDIT

There will be no extra credit assignments in this course.

## GRADING

During the semester, you will accumulate credits through your homework that will determine your homework performance grade. Problem sets will be graded by graduate student Madison Foreman.

If an answer is unintelligible or illegible, you will lose some or all credits for the problem. Late homework will not be graded and counts as zero credits, unless the late return is excused. Everyone may drop one homework assignment without penalty. Your total homework performance will count 40% towards the final grade.

At the end of the semester, your clicker points are summed and increased by 10% to allow for malfunctioning clickers and all other possible problems. These clicker points are then normalized to the maximum of achievable points. You will receive 1 clicker point per question, based on participation. However, recall that your honest and best response is what will help you and me – never click in just to click in. You'll learn much more – even if you're wrong – if you've given it your best effort. The participation in clicker questions will count 5% towards the final grade.

The average of the two-hour-exams will count 30% towards the final grade.

The final exam will count 25% towards the final grade.

## DATES WITHOUT CLASS MEETINGS

Due to conference or seminar travel, some class meetings may be canceled, but no concrete dates are planned so far. If necessary, some of the missed lectures may be given instead on other days or by a different instructor (to be announced). Up to two missed class meetings can be made up for in the midterm exams that are held outside of regular class hours.

## TENTATIVE LIST OF TOPICS

- 1) Classical Treatment of Interaction of Light and Matter
- 2) Transitions Between States - Einstein Coefficients
- 3) Line Shapes
- 4) States and Spectra of the H-Atom
- 5) States and Spectra of Multielectron Atoms
- 6) Orbit and Spin Magnetism, Spin-Orbit Interaction, Fine Structure
- 7) The Born-Oppenheimer Approximation
- 8) Purely Rotational Spectra of Diatomic Molecules
- 9) Ro-vibrational Spectra of Diatomic Molecules
- 10) Electronic States of Diatomic Molecules
- 11) Electronic Spectra of Diatomic Molecules
- 12) Multiphoton Transitions
- 13) Raman Spectroscopy
- 14) Nuclear Spin Statistics
- 15) Group Theory and Molecular Point Groups
- 16) Rotation of Polyatomic Molecules
- 17) Vibrations of Polyatomic Molecules
- 18) Electronic States of Polyatomic Molecules
- 19) Spectra of polyatomic molecules
- 20) Basics of Solid State Electronic Structure
- 21) Basics of Semiconductor Quantum Dot Electronic Structure

# SYLLABUS STATEMENTS

## CLASSROOM BEHAVIOR

Both students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in person, remote or online. Those who fail to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed, religion, sexual orientation, gender identity, gender expression, veteran status, political affiliation or political philosophy. For more information, see the policies on [classroom behavior](#) and the [Student Code of Conduct](#).

## REQUIREMENTS FOR COVID-19

As a matter of public health and safety due to the pandemic, all members of the CU Boulder community and all visitors to campus must follow university, department and building requirements, and public health orders in place to reduce the risk of spreading infectious disease. Required safety measures at CU Boulder relevant to the classroom setting include:

- maintain 6-foot distancing when possible,
- wear a face covering in public indoor spaces and outdoors while on campus consistent with state and county health orders,
- clean local work area,
- practice hand hygiene,
- follow public health orders, and
- if sick and you live off campus, do not come onto campus (unless instructed by a CU Healthcare professional), or if you live on-campus, please alert [CU Boulder Medical Services](#).

Students who fail to adhere to these requirements will be asked to leave class, and students who do not leave class when asked or who refuse to comply with these requirements will be referred to [Student Conduct and Conflict Resolution](#). For more information, see the policies on [COVID-19 Health and Safety](#) and [classroom behavior](#) and the [Student Code of Conduct](#). If you require accommodation because a disability prevents you from fulfilling these safety measures, please see the “Accommodation for Disabilities” statement on this syllabus.

All students who are new to campus must complete the [COVID-19 Student Health and Expectations Course](#). Before coming to campus each day, all students are required to complete the [Buff Pass](#).

Students who have tested positive for COVID-19, have symptoms of COVID-19, or have had close contact with someone who has tested positive for or had symptoms of COVID-19 must stay home. In this class, if you are sick or quarantined, and are registered for the in-person section of the course, please notify me immediately that you cannot come to class. If you are able to do so, you should participate remotely via the Zoom link given for the course.

## ACCOMMODATION FOR DISABILITIES

If you qualify for accommodations because of a disability, please submit your accommodation letter from Disability Services to your faculty member in a timely manner so that your needs can be addressed. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the [Disability Services website](#). Contact Disability Services at 303-492-8671 or [dsinfo@colorado.edu](mailto:dsinfo@colorado.edu) for further assistance. If you have a temporary medical condition, see [Temporary Medical Conditions](#) on the Disability Services website.

## PREFERRED STUDENT NAMES AND PRONOUNS

CU Boulder recognizes that students' legal information doesn't always align with how they identify. Students may update their preferred names and pronouns via the student portal; those preferred names and pronouns are listed on instructors' class rosters. In the absence of such updates, the name that appears on the class roster is the student's legal name.

## HONOR CODE

All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the Honor Code. Violations of the policy may include: plagiarism, cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty. All incidents of academic misconduct will be reported to the Honor Code ([honor@colorado.edu](mailto:honor@colorado.edu)); 303-492-5550). Students found responsible for violating the academic integrity policy will be subject to nonacademic sanctions from the Honor Code as well as academic sanctions from the faculty member. Additional information regarding the Honor Code academic integrity policy can be found at the [Honor Code Office website](#).

## SEXUAL MISCONDUCT, DISCRIMINATION, HARASSMENT AND/OR RELATED RETALIATION

The University of Colorado Boulder (CU Boulder) is committed to fostering an inclusive and welcoming learning, working, and living environment. CU Boulder will not tolerate acts of sexual misconduct (harassment, exploitation, and assault), intimate partner violence (dating or domestic violence), stalking, or protected-class discrimination or harassment by members of our community. Individuals who believe they have been subject to misconduct or retaliatory actions for reporting a concern should contact the Office of Institutional Equity and Compliance (OIEC) at 303-492-2127 or [cureport@colorado.edu](mailto:cureport@colorado.edu). Information about the OIEC, university policies, [anonymous reporting](#), and the campus resources can be found on the [OIEC website](#).

Please know that faculty and graduate instructors have a responsibility to inform OIEC when made aware of incidents of sexual misconduct, dating and domestic violence, stalking, discrimination, harassment and/or related retaliation, to ensure that individuals impacted receive information about options for reporting and support resources.

### RELIGIOUS HOLIDAYS

Campus policy regarding religious observances requires that faculty make every effort to deal reasonably and fairly with all students who, because of religious obligations, have conflicts with scheduled exams, assignments or required attendance. In this class, please indicate any such conflicts to me at least three weeks in advance of the conflicting date, preferably during the first week of classes. Religious observances on regular class dates do not constitute a problem, but please notify me as well about such occurrences.

See the [campus policy regarding religious observances](#) for full details.