

**Course:** CHEM 6300, Topics in Analytical Chemistry (Molecular and Analytical Spectroscopy), 3.0 credits

**Location:** T,R 13:15 – 14:30 (1:15 – 2:30 pm), HILLS AGRI SCI 235

**Instructor:** Prof. David Punahaole

**Office:** INNOVATION HALL E352

**Email:** [David.Punahaole@uvm.edu](mailto:David.Punahaole@uvm.edu)

**Office Hours:** TBD

**Prerequisite:** Graduate student

**Course Description:** In this course, you will learn the fundamental concepts and principles of optical spectroscopy methods of analysis. The course aims establish a rigorous foundation to understand fundamental aspects of different optical spectroscopies such as UV and IR absorbance, Rayleigh and Raman scattering, fluorescence, and select non-linear techniques. Emphasis will be placed on fundamental theoretical concepts, instrumentation, and applications in materials science, chemistry, biophysics, and imaging.

**Course Learning Objectives:** Upon the completion of this course, it is anticipated that you will be able to:

1. Describe the theories that underlie different optical methods.
2. Explain how different optical measurements are made and the instrumentation required.
3. Analyze spectroscopic data to extract information about molecular structural dynamics.
4. Critically evaluate literature in the field of molecular and analytical spectroscopy.

**Course Materials:** There is no required textbook for the course. However, several are recommended:

- Alan Marshall, *Biophysical Chemistry*, John Wiley & Sons, Inc. 1976
- Jeanne L. McHale, *Molecular Spectroscopy (1<sup>st</sup> or 2<sup>nd</sup> Ed.)*, CRC Press 2017
- James D. Ingle and Stanley R. Crouch, *Spectrochemical Analysis*, AbeBooks, 1988
- Max Diem, *Introduction to Modern Vibrational Spectroscopy*, John Wiley & Sons, Inc. 1993
- Robert W. Boyd, *Nonlinear Optics (3<sup>rd</sup> Ed.)*, Academic Press, Inc. 2008

Copies of the chapters belonging to these textbooks can be made available upon request to me. These copies are for educational purposes only. Please do not distribute these copies.

**Web Content:** Lecture notes, problem sets, problem set answer keys, and exams may be made available through Brightspace. These materials are available for all current, UVM-affiliated, students, but they may not be shared off-campus without permission of the instructor.

**Attendance Policy:** Attendance will not be taken for this course, but you are expected to attend all lectures to do well. If you miss a lecture for any reason, it is your responsibility to catch-up on missed material.

**Grading:** Grades will follow the standard UVM scale:

- A+: >96 – 100%
- A: >92 – 96%
- A-: >89 – 92%
- B+: >87 – 89%
- B: >82 – 86%
- B-: >79 – 82%
- C+: >76 – 79%
- C: >72 – 76%
- C-: >69 – 72%
- D+: >66 – 69%
- D: >62 – 66%
- D-: >60 – 62%
- F: <60%

**Graded Components:**

- *Exams (50%):* two exams are scheduled for this course. They will each be worth 25% of your final grade. They are not cumulative, although the questions from the exams will draw upon concepts discussed throughout the course.
- *Problem Sets (25%):* A total of 5 problem sets will be assigned throughout the semester. Each problem set is worth 5% of your total grade. Problem sets will be due at the start of class on the due date listed. Submissions that are late due to illegitimate reasons will not be accepted.
- *Class Discussions (25%):* Students will engage in a group discussion based on a paper selected by me.

**Statement on Diversity and Inclusion:** I strive to create a classroom environment that supports students from a diverse set of backgrounds. Our society is composed of individual from diverse ethnic, socioeconomic, and educational backgrounds. Half of our society are women. I strongly believe that our best path forward to a stronger and more equitable society is to promote inclusiveness. It is my expectation that every member of this class will also support diversity and inclusion. As a community, we should strive to uphold the ideals of Our Common Ground: <https://www.uvm.edu/president/our-common-ground>. I welcome any suggestions as to how I can promote a diverse and inclusive classroom.

**General statement regarding potential changes during the semester:** <http://catalogue.uvm.edu/> The University of Vermont reserves the right to make changes in the course offerings, mode of delivery, degree requirements, charges, regulations, and procedures contained herein as educational, financial, and health, safety, and welfare considerations require, or as necessary to be compliant with governmental, accreditation, or public health directives.

**Green and Gold Promise:** The Green and Gold Promise clearly articulates the expectations that UVM has for students, faculty, and staff to remain compliant with all COVID-19 recommendations from the federal CDC, the State of Vermont, and the City of Burlington. The Code of Student Conduct outlines policies related to violations of the Green and Gold Promise. Sanctions for violations include fines, educational sanctions, parent notification, probation, and suspension.

**Intellectual Property Statement/Prohibition on Sharing Academic Materials:** Students are prohibited from publicly sharing or selling academic materials that they did not author (for example: class syllabus, outlines or class presentations authored by the professor, practice questions, text from the textbook or other copyrighted class materials, etc.); and students are prohibited from sharing assessments (for example homework or a take-home examination). Violations will be handled under UVM's Intellectual Property policy and Code of Academic Integrity.

**Student Learning Accommodations:** In keeping with university policy, any student with a documented disability interested in utilizing accommodations should contact SAS, the office of Disability Services on campus. SAS works with students and faculty in an interactive process to explore reasonable and appropriate accommodations, which are communicated to faculty in an accommodation letter. All students are strongly encouraged to meet with their faculty to discuss the accommodations they plan to use in each course. A student's accommodation letter lists those accommodations that will not be implemented until the student meets with their faculty to create a plan.

**Contact SAS:**

A170 Living/Learning Center  
802-656-7753  
access@uvm.edu  
[www.uvm.edu/access](http://www.uvm.edu/access)

**Religious Holidays:** Students have the right to practice the religion of their choice. If you need to miss class to observe a religious holiday, please submit the dates of your absence to me in writing by the end of the second full week of classes. You will be permitted to make up work within a mutually agreed-upon time. <https://www.uvm.edu/registrar/religious-holidays>.

**Academic Integrity:** The policy addresses plagiarism, fabrication, collusion, and cheating. <https://www.uvm.edu/policies/student/acadintegrity.pdf>.

**Grade Appeals:** If you would like to contest a grade, please follow the procedures outlined in this policy: <https://www.uvm.edu/policies/student/gradeappeals.pdf>.

**Code of Student Conduct:** <http://www.uvm.edu/policies/student/studentcode.pdf>

**FERPA Rights Disclosure:** The purpose of this policy is to communicate the rights of students regarding access to, and privacy of their student educational records as provided for in the Family Educational Rights and Privacy Act (FERPA) of 1974. <http://catalogue.uvm.edu/undergraduate/academicinfo/ferparightsdisclosure/>

**Promoting Health & Safety:** The University of Vermont's number one priority is to support a healthy and safe community:

**Center for Health and Wellbeing**  
<https://www.uvm.edu/health>

**Counseling & Psychiatry Services (CAPS)**  
Phone: (802) 656-3340

**C.A.R.E.**

If you are concerned about a UVM community member or are concerned about a specific event, we encourage you to contact the Dean of Students Office (802-656-3380). If you would like to remain anonymous, you can report your concerns online by visiting the Dean of Students website at <https://www.uvm.edu/studentaffairs>.

**Final Exam Policy:** The University final exam policy outlines expectations during final exams and explains timing and process of examination period. <https://www.uvm.edu/registrar/final-exams>.

**Statement on Alcohol and Cannabis in the Academic Environment:** As a faculty member, I want you to get the most you can out of this course. You play a crucial role in your education and in your readiness to learn and fully engage with the course material. It is important to note that alcohol and cannabis have no place in an academic environment. They can seriously impair your ability to learn and retain information not only in the moment you may be using, but up to 48 hours or more afterwards. In addition, alcohol and cannabis can:

- Cause issues with attention, memory and concentration
- Negatively impact the quality of how information is processed and ultimately stored
- Affect sleep patterns, which interferes with long-term memory formation

**It is my expectation that you will do everything you can to optimize your learning and to fully participate in this course.**

**Course Schedule****Week 1, 08/28 – 09/1**

- Lecture 1: Syllabus introduction, harmonic oscillator
- Lecture 2: Introduction to electromagnetism, properties of light

**Week 2, 09/04 – 09/08**

- Lecture 3: Electrostatics, dipole moment, polarizability
- Lecture 4: Classical Theory of absorption and dispersion

**Week 3, 09/11 – 09/15**

- Lecture 5: Time-dependent perturbation theory
- Lecture 6: Spectral lineshapes and dynamics

**Week 4, 09/18 – 09/22**

- Lecture 7: Relationship between refractive index, polarizability, and permittivity
- Lecture 8: Electronic absorption and emission (fluorescence) spectroscopy

**Week 5, 09/25 – 09/29**

- Lecture 9: Absorption/Fluorescence Instrumentation
- Lecture 10: Absorption/Fluorescence Applications

**Week 6, 10/02 – 10/06**

- Lecture 11: Vibrational normal modes
- EXAM 1

**Week 7, 10/09 – 10/13**

- NO CLASSES

**Week 8, 10/16 – 10/20**

- Lecture 12: How vibrations report on structural dynamics and interactions
- Lecture 13: Infrared Spectroscopy theory

**Week 9, 10/23 – 10/27**

- Lecture 14: FTIR, ATR, Photothermal IR
- Lecture 15: Rayleigh and Raman scattering

**Week 10, 10/30 – 11/03**

- Lecture 16: Resonance Raman scattering: Vibronic theory
- Lecture 17: Surface and Tip-enhanced Raman Spectroscopy

**Week 11, 11/06 – 11/10**

- Lecture 18: Raman Instrumentation
- Lecture 19: Applications of IR and Raman spectroscopy

**Week 12, 11/13 – 11/17**

- Lecture 20: Classical theory of non-linear optical processes
- Lecture 21: Second harmonic and sum frequency generation

**Week 13, 11/20 – 11/24**

- THANKSGIVING BREAK, NO CLASSES

**Week 14, 11/27 – 12/01**

- Lecture 22: Introduction to Coherent Raman Spectroscopy
- Lecture 23: Coherent Raman Instrumentation

**Week 15, 12/04 – 12/08**

- Lecture 24: Coherent Raman Applications
- EXAM 2