Molecular Spectroscopy

CHM 67605 (CRN 20984, 3 credits), Fall 2020

1:30 PM - 2:20 PM	**Mon/Wed**	**BRWN 3104**
1:30 PM - 2:20 PM	**Fri**	**SC G046**

Web access:

- **Brightspace:** https://purdue.brightspace.com/d2l/home/52483
- **nanoHUB:** https://nanohub.org/tools/molspec

Instructor Contact:
Mike Reppert
E-mail: reppertm@purdue.edu
Office: BRWN 4171D
Office hours: **Online** or by appointment
Phone: 765-494-2064
Preferred contact method: e-mail

Course Description:
This course offers an overview of fundamental theory and applications in optical and infrared spectroscopy. Topics addressed will include: electrodynamics, response theory, linear and nonlinear experimental methods (including two-dimensional spectroscopy), density matrix dynamics, harmonic and excitonic molecular models, dephasing and decoherence.

Expected learning outcomes include:

- An *intuitive* understanding of the physical principles behind molecular spectroscopy,
- A basic familiarity with both classical and modern experimental spectroscopic techniques, and
- The computational skills (particularly in Python programming) needed to process experimental spectroscopic data and to build and test simple physical models.

Learning Resources, Technology, and Texts:

- **No textbook** is required for this course. As a reference, however, some students may find Becker's textbook useful:

  > Richard Becker, *Electromagnetic Fields and Interactions, vols. 1-2.* Available from Dover Books on Physics.

- An **online textbook** covering much of the course material is hosted at the Instructor's homepage.
- The course **Brightspace page** will be used for homework submission/grading and online office hours (via the "Virtual Classroom" tool).
- A dedicated **nanoHUB page** hosts the course schedule and links to lecture notes and interactive, Jupyter Notebook-based notes, tutorials, and exercises.

Exercises and Grading:

Grades for the course will be determined on a 100 pt grading scale distributed between weekly exercises, two mid-term exams, and a final project as listed in the following table.

Assignment	Due	Points
Exercises	Weekly	48
Midterm 1	Sep 25	16
Midterm 2	Oct 30	16
Final Project	Dec 4	20

- Exercises will typically be assigned at or before Friday lecture and will be due the following Friday. All exercises should be submitted as Jupyter Notebook (*.ipynb) files on Brightspace. Late assignments will be assigned a 1% penalty for every *hour* past the deadline. For example, an exercise due at midnight and submitted at 1 AM will be penalized 1%; an exercise submitted 24 hours late will be penalized 24%. No credit will be assigned for exercises turned in more than 100 hours (roughly four days) late. Grading may be delayed for late assignments.
- At present, both midterm exams are scheduled to be administered during the normal class meeting time. If necessary to allow for remote work, these may be switched to take-home exams.
- The final project will consist of a coding assignment, presentation (delivered to the class), and a brief ($<$ 5 pages) write-up on a method or technique in molecular spectroscopy chosen by the student. Write-up and code will be due the last day of classes. In-person presentations will be scheduled in normal class periods near the end of the semester.

Letter grades will be assigned according to the total number of points as follows:

- **A**: $\geq$ 90 pts
- **B**: $\geq$ 80 pts
- **C**: $\geq$ 70 pts
- **D**: $\geq$ 50 pts
- **F**: $<$ 50 pts

Opportunities for extra credit will be made available throughout the semester.

Tips for Success:

- Ask questions! The best way to get clarification on a concept is to ask for it.
- Start work on assignments *right away*. Some problems will require some time to think about your approach.
- Be willing to "speak up" if problems arise.
- Come to office hours. (If you have a conflict, let the instructor know in advance.)

Teaching Philosophy:

I view science as an exploratory quest. My role as an instructor is to guide our expedition into territory that you've most likely seen in the distance but not close at hand. Although I've passed this way before, there are many features to the landscape that I've never observed in detail. Collectively, our goal is to become more familiar with the terrain and to establish individual base camps for future exploration. Exams, assignments, and especially the final project are your opportunities to strike out on your own, in preparation for independent travel.

Attendance:

All students are expected to regularly attend lectures. However, compliance with this policy is the responsibility of the individual student: no regular attendance records will be taken, and attendance will not be used to determine grades.

Students should stay home and contact the Protect Purdue Health Center (496-INFO) if they feel ill, have any symptoms associated with COVID-19, or suspect they have been exposed to the virus. In the current context of COVID-19, in-person attendance will not be a factor in the final grades, but the student still needs to inform the instructor of any conflict that can be anticipated and will affect the submission of an assignment or the ability to take an exam. Only the instructor can excuse a student from a course requirement or responsibility. When conflicts can be anticipated, such as for many University-sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible. For unanticipated or emergency conflict, when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, through Brightspace, or by phone. When the student is unable to make direct contact with the instructor and is unable to leave word with the instructor's department because of circumstances beyond the student's control, and in cases of bereavement, quarantine, or isolation, the student or the student's representative should contact the Office of the Dean of Students via email or phone at 765-494-1747. Our course Brightspace includes a link on Attendance and Grief Absence policies under the University Policies menu.

Academic Integrity:

Specific expectations for this course: Students are expected and encouraged to work together on exercises (while respecting social distancing guidelines!). However, the work submitted by each student is expected to be their own. Electronic submissions (e.g., computer code) are expected to have been manually written by each student individually. Copy-and-pasting work from other students constitutes a violation of the honor code. Copy-and-pasting code *provided by the instructor* as part of the assignment or any other exercise *is* permitted. No collaboration, or communication with other students is allowed during exams unless explicitly stated in writing by the instructor.

University Policy: "Academic integrity is one of the highest values that Purdue University holds. Individuals are encouraged to alert university officials to potential breaches of this value by either emailing integrity@purdue.edu or by calling 765-494-8778. While information may be submitted anonymously, the more information that is submitted provides the greatest opportunity for the university to investigate the concern."

Consequences: Incidents of academic misconduct in this course will be addressed by the course instructor and referred to the Office of Student Rights and Responsibilities (OSRR) for review at the university level. Any violation of course policies as it relates to academic integrity will result minimally in a failing or zero grade for that particular assignment, and at the instructor's discretion may result in a failing grade for the course. In addition, all incidents of academic misconduct will be forwarded to OSRR, where university penalties, including removal from the university, may be considered.

Honor Pledge: "As a boilermaker pursuing academic excellence, I pledge to be honest and true in all that I do. Accountable together – we are Purdue."

Academic Guidance in the Event a Student is Quarantined/Isolated:

If you become quarantined or isolated at any point in time during the semester, in addition to support from the Protect Purdue Health Center, you will also have access to an Academic Case Manager who can provide you academic support during this time. Your Academic Case Manager can be reached at acmq@purdue.edu and will provide you with general guidelines/resources around

communicating with your instructors, be available for academic support, and offer suggestions for how to be successful when learning remotely. Importantly, if you find yourself too sick to progress in the course, notify your academic case manager and notify me via email or Brightspace. We will make arrangements based on your particular situation. The Office of the Dean of Students (odos@purdue.edu) is also available to support you should this situation occur.

Classroom Guidance Regarding Protect Purdue:

The Protect Purdue Plan, which includes the Protect Purdue Pledge, is campus policy and as such all members of the Purdue community must comply with the required health and safety guidelines. Required behaviors in this class include: staying home and contacting the Protect Purdue Health Center (496-INFO) if you feel ill or know you have been exposed to the virus, properly wearing a mask in classrooms and campus building, at all times (e.g., mask covers nose and mouth, no eating/drinking in the classroom), disinfecting desk/workspace prior to and after use, maintaining appropriate social distancing with peers and instructors (including when entering/exiting classrooms), refraining from moving furniture, avoiding shared use of personal items, maintaining robust hygiene (e.g., handwashing, disposal of tissues) prior to, during and after class, and following all safety directions from the instructor.

Students who are not engaging in these behaviors (e.g., wearing a mask) will be offered the opportunity to comply. If non-compliance continues, possible results include instructors asking the student to leave class and instructors dismissing the whole class. Students who do not comply with the required health behaviors are violating the University Code of Conduct and will be reported to the Dean of Students Office with sanctions ranging from educational requirements to dismissal from the university.

Any student who has substantial reason to believe that another person in a campus room (e.g., classroom) is threatening the safety of others by not complying (e.g., not wearing a mask) may leave the room without consequence. The student is encouraged to report the behavior to and discuss next steps with their instructor. Students also have the option of reporting the behavior to the Office of the Student Rights and Responsibilities. See also Purdue University Bill of Student Rights.

Nondiscrimination:

Purdue University is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life. Purdue's nondiscrimination policy can be found at `http://www.purdue.edu/purdue/ea_eou_statement.html`.

Accessibility:

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: drc@purdue.edu or by phone: 765-494-1247. More details are available on our course Brightspace under Accessibility Information.

Mental Health:

- If you find yourself beginning to feel some stress, anxiety, and/or feeling slightly overwhelmed, try WellTrack, https://purdue.welltrack.com. Sign in and find information and tools at your fingertips, available to you at any time.

- If you need support and information about options and resources, please contact or see the Office of the Dean of Students. Call 765-494-1747. Hours of operation are M-F, 8 am- 5 pm.
- If you find yourself struggling to find a healthy balance between academics, social life, stress, etc. sign up for free one-on-one virtual or in-person sessions with a Purdue Wellness Coach at RecWell. Student coaches can help you navigate through barriers and challenges toward your goals throughout the semester. Sign up is completely free and can be done on BoilerConnect. If you have any questions, please contact Purdue Wellness at evans240@purdue.edu.
- If you're struggling and need mental health services: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at (765)494-6995 and during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

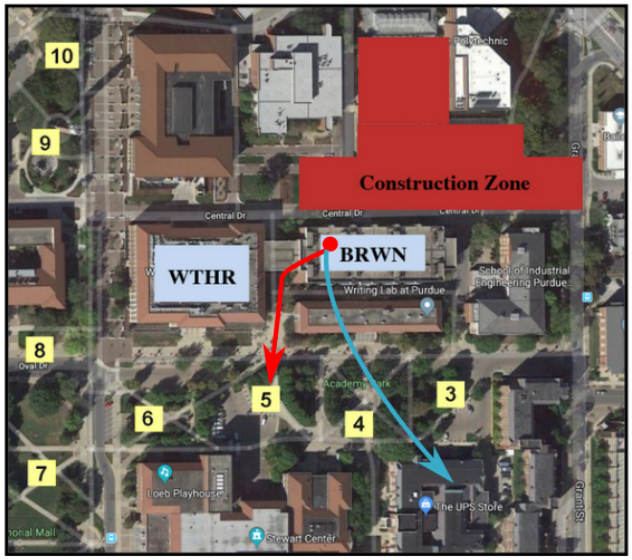
Emergency Preparation:

Emergency preparedness is your personal responsibility. Purdue University is actively preparing for natural disasters or human-caused incidents with the ultimate goal of maintaining a safe and secure campus. Let's review the following procedures:

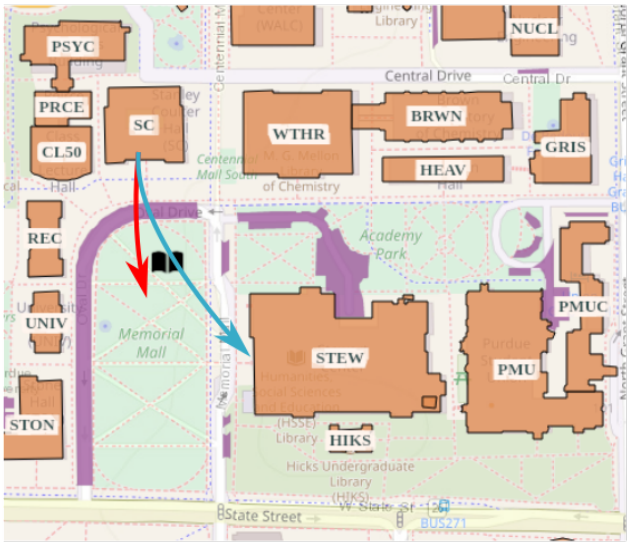
- For any emergency call 911.
- There are nearly 300 Emergency Telephone Systems throughout campus that connect directly to the Purdue Police Department (PUPD). If you feel threatened or need help, push the button and you will be connected to the PUPD.
- If we hear a fire alarm we will immediately evacuate the building and proceed to one of the Emergency Assembly Areas marked on the maps below. **Do not use the elevator**.
- If we are notified of a Shelter in Place requirement for a tornado warning we will shelter in the lowest level of this building away from windows and doors. Our preferred location is the BRWN basement hallway (directly downstairs from this classroom) or the SC basement hallway just outside the classroom (away from all external windows and doors).
- If we are notified of a Shelter in Place requirement for an active threat such as a shooting we will shelter in a room that is securable preferably without windows. Our preferred location is any securable room on this floor.
- If we are notified of a Shelter in Place requirement for a hazardous materials release we will shelter in our classroom shutting any open doors and windows.

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.

EMERGENCY ASSEMBLY AREAS (EAA's)



Your Location	EAA
BRWN 1st	#3
BRWN 2nd	#4
BRWN 3rd	#5
BRWN 4th & 5th	#3
BRWN Basement	#4
WTHR 200 class	#7
WTHR 1st & 2nd	#8
WTHR 3rd	#6
WTHR 4th & 5th	#10
WTHR Basement	#9



Default

Inclement Weather

EMERGENCY	SHELTER IN PLACE OPTIONS FOR CONSIDERATION
Weather-Related - Tornado Warning	Basement corridors, basement offices, basement restrooms Or the lowest level of the building (stay away from windows and doors)
Hazardous Materials (HAZMAT) Release	Remain or find an unaffected office or work area and close windows and doors.
Active threat, such as a shooting	Seek a safe location, preferable a room without windows that can be locked or secured by barriers.