CHEM 401/501 – Advanced Physical Chemistry
Fall 2022 Syllabus

Instructor: Prof. Nathanael M. Kidwell
Office: ISC 1287, (757)221-1701
Email: nmkidwell@wm.edu
Office Hours: W 4:30 - 5:30 pm; or by appointment or drop by

Course Information
Class Meetings: TR 3:30 - 4:50 pm
Class Location: ISC 1280
Website: Course information will be posted on Blackboard

Diversity & Inclusion Vision Statement
The College of William & Mary values and actively nurtures an environment of diversity and inclusiveness where every individual, regardless of how we may differ – for example, but not limited to, with regard to race, religion, gender, ethnic origin, age, socioeconomic status, political preferences, physical abilities, or sexual orientation – is embraced, respected, and afforded the same opportunity to grow, to succeed, and to contribute to William & Mary's success.

Student Accessibility Services
William & Mary accommodates students with disabilities in accordance with federal laws and university policy. Any student who feels they may need an accommodation based on the impact of a learning, psychiatric, physical, or chronic health diagnosis should contact Student Accessibility Services staff at 757-221-2509 or at sas@wm.edu to determine if accommodations are warranted and to obtain an official letter of accommodation. For more information, please see www.wm.edu/sas.

Course Description and Goals
In this course, we will focus on advanced topics in quantum chemistry, molecular spectroscopy, chemical dynamics, atmospheric chemistry, modern experimental physical chemistry, and other selected topics. Linking material learned in class to modern physical chemistry techniques and research will be highlighted to give you opportunities to see how Physical Chemists are solving current, real-world problems. Class meetings will be a mixture of lecture, discussion, workshops, and student presentations.

Text
Links to the E-books are available through the Swem Library website. Other supplemental resources will be posted on Blackboard.

(1) *Spectra of Atoms and Molecules, 2nd Edition* by Peter Bernath; Oxford University Press, 2005. ISBN: 0-19-517759-2.

(2) *Molecular Reaction Dynamics* by Raphael D. Levine; University Science Books, 2005. ISBN: 0-521842-76-X.

Deadlines

Add/Drop Deadline: 09/12
Withdraw Deadline: 10/31

Course Structure and Grading

Research Grant Proposal (50%)

A major component of this course involves a semester-long research project where you will become an expert in an active research area in the top Ph.D. programs in physical chemistry. *The overarching goals of the project are to: learn advanced physical chemistry concepts and the current state of the field, develop problem-solving skills, gain experience in the peer review and response process, enhance written and oral communication skills, and synthesize information to propose a novel research direction.* CHEM 401 students may work in pairs. CHEM 501 students must complete a project individually. Projects will culminate in a research grant proposal (paper) and class presentation, though there are several scaffolded "deliverables" along the way. These activities include developing writing skills in a "process," evaluating the work of your peers, composing a response to reviewers, and creating effective presentation slides – all of which play an important role in manuscript and grant writing process as well as professional presentations. Over the course of the semester, students will generate a research grant proposal that will be turned in at the end of the semester. A complete description of the research grant proposal project with point breakdown is included on page 9 of this syllabus.

Problem Sets (20%)

There is no better way to master Physical Chemistry than by solving problems. Therefore, several graded problem sets will be posted on Blackboard due in class on the specified date. Late work (without approval from instructor) will lose 5 points. Problem sets turned in after the last day of class will not be graded. Working together in study groups is encouraged as a helpful and enjoyable way to overcome conceptual obstacles and share the satisfaction of gained understanding. At the heart of good science is collaboration, so work together with your colleagues to solve problems. However, to facilitate the development of independent problem-solving skills, problem sets must be completed and submitted individually. Problem sets will be graded for completion and accuracy, and solutions made available on Blackboard.

Mid-Term Exam (20%)

The mid-term is a take-home exam. The mid-term exam is open note (handouts, problem sets, textbooks, and Blackboard materials), but using additional resources (i.e., the internet, other students, publications, etc.) is not permitted. The take-home mid-term exam is due one week after distribution. The mid-term exam is due: 5 pm on Thursday, Oct. 27th.

Class Participation (10%)
In this course, we will learn about the principles and applications of molecular spectroscopy and chemical dynamics. In order for our class discussions to be meaningful, it is essential that you are prepared and participating in the day's topic. Full participation includes coming to class prepared, asking and answering questions, sharing in discussion, collaborating and communicating effectively with your peers, and delivering presentations.

To receive a grade in the A range in this course, you must have at least 90%; the B range is at least 80%; the C range is at least 70%, and the D range is at least 60%. These thresholds may be lowered (i.e., it may become easier to get a higher grade), but they will not be raised.

Policies

Email: I will make every effort to respond to emails promptly. **When you email me, please put CHEM 401/501 in the subject line.** In order to encourage you to proactively prepare for exam and problem set due dates, I reserve the right not to answer last minute emails that are received after 5:00 pm the night before an exam or problem set due date.

Make-up Policy: No make-up assignments will be given without (a) pre-arranging this with me **well before** the day of the exam **OR** (b) providing documentation demonstrating a medical emergency. No extensions will be given for problem sets. **I am prepared to be flexible with these policies to a reasonable degree if you are significantly impacted by COVID-19. Extenuating circumstances must be communicated to me in a timely manner.**

Tentative Order of Topics

Molecular Spectroscopy Topics

I. An Overview of Molecular Spectroscopy (Ch. 1, Bernath)

a. Nature of electromagnetic radiation
b. The components of a spectrum: frequencies, intensities, lineshapes
c. Mechanisms of line broadening
d. Molecular symmetry: A first look (Ch. 2, Bernath)

II. Vibrational Spectroscopy of Diatomics (Ch. 7.1, Bernath)

a. Infrared selection rules in the H.O. approximation
b. Anharmonicity, Vibration-rotation coupling

III. Point Group Theory (Ch. 3, 4, Bernath)

1. Some fundamentals

a. Matrix representations of a group, irreducible matrix representations, similarity transformations, reduction of a reducible matrix representation projection operators and direct products

2. Applying group theory to spectroscopy

a. The symmetries of rotations, vibrations, electronic states
b. Selection rules

IV. Vibrational Spectroscopy of Polyatomics (Ch. 7, 8, Bernath)

a. Vibrational symmetries, Normal mode analysis
b. IR and Raman selection rules
c. Vibration-rotation spectroscopy of polyatomics, Local modes
d. Large-amplitude motions:
Internal rotation, inversion, tunneling, molecular symmetry groups
e. Intramolecular vibrational redistribution (IVR)

V. Electronic Spectroscopy of Diatomics (Ch. 9, Bernath)

a. Term symbols, Selection rules
b. Franck-Condon factors, Predissociation

VI. Electronic Spectroscopy of Polyatomics (Ch. 10, Bernath)

a. Electronic selection rules
b. Polyatomic Franck-Condon Analysis
c. Duschinsky mixing
d. Vibronic coupling: Herzberg-Teller, Renner-Teller, Jahn-Teller

Chemical Dynamics Topics

I. Understanding Chemical Reactions at the Molecular Level (Ch. 1, Levine)

a. What is molecular reaction dynamics?
b. An example: energy disposal in an exoergic chemical reaction

II. Molecular Collisions

a. Simple collision processes (pp. 36-44, Levine)
b. Reaction cross section (pp. 75-79, Levine)
c. Opacity function (pp. 84-89, Levine)
d. Classical scattering (pp. 109-116, Levine)

III. Introduction to Polyatomic Dynamics (Ch. 5, Levine)

a. Potential energy functions and chemical reactions
b. The classical trajectory approach to reaction dynamics
c. Energy and dynamics of the chemical change

IV. Structural Considerations in the Calculation of Reaction Rates (Ch. 6, Levine)

a. Transition state theory: The rate of barrier crossing
b. Density of states and partition functions
c. Roaming mechanism
d. RRKM theory and the rate of unimolecular reactions
e. Resolving final states and populations
f. Characterization of energy disposal and energy requirements of chemical reactions

V. Photoselective chemistry: Access to the transition state region (Ch. 7, Levine)

a. Franck-Condon principle, Beyond the B.O. approximation,
Radiationless transitions, The Picket Fence model
b. Laser photoexcitation and photodetection of diatomic molecules
c. Photodissociation dynamics

Research Grant Proposal

List of Possible Principal Investigators (PIs):

Anne McCoy (Washington) – vibrational spectroscopy, theory, atmosphere
Krupa Ramasesha (Sandia Nat'l Labs) – ultrafast dynamics, energy
Marissa Weichman (Princeton) – spectroscopy, nanoscience
Michael Heaven (Emory) – electronic spectroscopy, chemical bonding
Michael Duncan (Georgia) – spectroscopy, dynamics, organometallics
Laura McCaslin (Sandia Nat'l Labs) – dynamics, energy, atmosphere
Daniel Neumark (UC-Berkeley) – spectroscopy, dynamics, atmosphere
Simon North (Texas A&M) – dynamics, atmosphere, astrochemistry
Mitchio Okumura (Caltech) – spectroscopy, astrochemistry
Renee Frontiera (Minnesota) – ultrafast spectroscopy, plasmonics, biology
Edwin Sibert (Wisconsin-Madison) – vibrational spectroscopy, theory
John Stanton (Florida) – spectroscopy, theory, chemical kinetics
Jingsong Zhang (UC-Riverside) – dynamics, atmosphere, chemical kinetics
Millard Alexander (Maryland) – dynamics, molecular collisions
Anna Krylov (Southern California) – spectroscopy, theory, solar, bioimaging
Robert Continetti (UC-San Diego) – dynamics, environmental
Gary Douberly (Georgia) – vibrational spectroscopy, astrochemistry
Joseph Francisco (Penn)- spectroscopy, theory, atmosphere
Etienne Garand (Wisconsin-Madison) – spectroscopy, catalysis
Christopher Johnson (Stony Brook) – spectroscopy, atmosphere, catalysis
Scott Kable (New South Wales) – spectroscopy, atmosphere
Marsha Lester (Penn) – vibrational spectroscopy, dynamics, atmosphere
Andrew Orr-Ewing (Bristol) – ultrafast spectroscopy, atmosphere, aerosols
David Osborn (Sandia Nat'l Lab) – spectroscopy, energy, atmosphere
Craig Murray (UC-Irvine) – spectroscopy, dynamics, atmosphere
Hanna Reisler (Southern California) – dynamics, atmosphere, energy
Timothy Schmidt (New South Wales) – spectroscopy, astrochemistry, solar
Lyudmila Slipchenko (Purdue) – spectroscopy, theory
Arthur Suits (Missouri) – dynamics, astrochemistry
Craig Taatjes (Sandia Nat'l Lab) – kinetics, energy, atmosphere
Claire Vallance (Oxford) – dynamics, atmosphere, astrochemistry
Bas van de Meerakker (Radboud University, Nijmegan) – dynamics, energy
J. Mathias Weber (Colorado) – spectroscopy, energy, nanomaterials
David Nesbitt (Colorado) – spectroscopy, nanomaterials, biophysics
David Yarkony (Johns Hopkins) – dynamics, photochemistry, energy
Hua Guo (New Mexico) – dynamics, energy, atmosphere
Knut Asmis (Leipzig) – vibrational spectroscopy, biology
Caroline Jarrold (Indiana) – dynamics, energy, environment
Scott Reid (Marquette) – dynamics, spectroscopy, atmosphere, combustion
Jinjun Liu (Louisville) – spectroscopy, atmosphere
Henry Schaeffer III (Georgia) – spectroscopy, theory, biology, atmosphere
Richard Zare (Stanford) – spectroscopy, nanoscience, green synthesis
Mark Johnson (Yale) – spectroscopy, atmosphere, catalysis

IMPORTANT: All paper assignments must have a unique title, 1" paper margins, page numbers, 1.5 line spacing, 11- or 12-pt. font (Times New Roman/Arial or similar). Figures (when necessary for clarity) must be legible, include captions with salient citations, and not exceedingly large. Grading rubrics for major components will be posted to Blackboard in advance of the assignment deadline.

Timeline of Events:

1. *Workshop: Research & Citation Tools.* In this workshop you will work toward gathering salient, high-quality, reputable sources for your research grant proposal (paper) and presentation. You will learn how to use reference management software and cite in ACS format. (*Cox Classroom, Swem Library on 9/20*)

2. *Choose 2 PIs (~1 page):* Investigate the PIs listed above (**and others if you wish**). Find publications on their website and SciFinder to find journal articles. Students (individuals or teams as appropriate) will submit a ranked list of their top 2 choices along with the citation (use ACS format) of one research article from each PI on which they plan to focus. Topics must be relevant to the course material and not too closely related to your current research. Include a brief justification of your choices (career plans, relationship to course material, research interests/experience, etc.) (*Due to Blackboard by 9/27*)

3. *Annotated Bibliography (~5 pages):* Once PI assignments are finalized, you will have ~2 weeks to pursue an in-depth study of their publications. There are hundreds, if not thousands, of manuscripts related to your topic – careful thought must be devoted to focusing on 3 related papers that can be combined to tell a compelling story. One of these papers should be a high-quality review – a "primer" article that covers the fundamentals/theory/applications of the research area. You may choose letters/communications, but at least one article must be a full-length manuscript in a high-quality peer-reviewed journal (e.g., *J. Phys. Chem.*). You will need additional literature sources to successfully complete the paper, which the tools at the Swem research workshop should help you find. Please see me with any questions/concerns. Submit an annotated bibliography that describes the overall proposed topic (this section contains the makings of your future thesis statement) as well as summarizes, assesses, and reflects the sources. Use correct ACS citation format: in-text citations as superscript numbers and a complete bibliography. A useful resource on annotated bibliographies can be found here: https://owl.english.purdue.edu/owl/resource/614/1/. (*Due to Blackboard by 10/11*)

4. *Create & Revise a Slide Assignment*: This assignment is designed to aid in your preparation for your final presentation. Individuals will create one slide for their final presentation. Next, after watching Jean-luc Doumont's video *Creative Effective Slides* and answering a few questions, individuals will then revise their slide to be consistent with his design principles. (*Due to Blackboard by 11/1*) Time permitting: your peers will evaluate the revised slide in class.

5. *Research Grant Proposal "Draft":* Submit two copies of a "draft" of the 7-8 page (not including references) research grant proposal (paper). *In addition to the background information included to describe previous work, the research grant proposal "draft" and final versions should also include a "next research direction" element that incorporates a research hypothesis objective, the planned methodology, and the appropriateness of the technique to address the hypothesis.* One copy should not contain your name. The draft must not be a first draft. Ask a classmate to read and thoughtfully edit it before submission or make a free appointment with the Writing Resource Center (WRC). Submit the name of one or more of your peers in CHEM 401/501 who has already reviewed this paper or indicate that it was reviewed at the WRC. Frequent grammatical and spelling errors in a draft are unacceptable – they will lead to a poor evaluation from your peers and me. A grading rubric for the draft will be posted in advance of the deadline. (*Due in class on 11/10*)

6. *Peer Review a Paper:* Individuals will complete an anonymous peer review of a randomly-selected paper. You will submit a copy of the paper with your written comments as well as the completed peer review form. (*Due in class on 11/17*)

7. *Practice Presentation & Peer Feedback:* Students will create and deliver a practice presentation to a group of peers using Doumont's design principles. A rubric will be posted to Blackboard to guide the design and creation of your materials and delivery. Peer review forms from the workshop are due within 24 hours of the talk - your scores will be based on the extent of your thorough and constructive feedback. (*In class on 11/22*)

8. *Class Presentation and Discussion:* Present a 20-30 minute talk on your research topic, followed by a 5-minute discussion period. Students will be evaluated on the quality, style, and content of their talk as well as the level of class participation. Students must email me the .pptx or .pdf file no later than 8 AM the day of your presentation so that I can print class handouts. (*In class between 12/1 and 12/8*)

9. *Research Grant Proposal Portfolio:* Submit the complete research grant proposal portfolio (organized in one binder or folder) that contains all materials previously submitted, the peer reviews of your paper, a final version of the research grant proposal, a 1-2 paragraph "Response to Reviewers" that explains how the reviewer comments (made by me and your peers) were addressed (what was the big-picture take home and how you addressed it). Also submit a digital copy of the final paper on Blackboard. Finally, a self/group evaluation form must be completed and turned in with the portfolio. (*Due in class and to Blackboard by 12/14 by 5pm*)

Research Grant Proposal Points Breakdown:
1. Choose Two PIs (10 pts)
2. Annotated Bibliography (30 pts)
3. Create & Revise a Slide (15 pts)
4. Research Grant Proposal "Draft" (50 pts)
5. Peer Review a Paper (15 pts)
6. Practice Presentations & Peer Feedback (30 pts)
7. Class Presentations and Discussion (75 pts)
8. Response to Reviewers (15 pts)
9. Final Research Grant Proposal (75 pts)
10. Self/Group Evaluation (10 pts)
Total = 325 pts (50% of final grade)

Date	Important Dates
	Add/Drop ends 9/12
9/20	Workshop: Research and Citation Tools (Meet in the Cox Classroom in Swem Library)
9/22	**Problem Set 1 Due**
9/27	Choose 2 PIs Due
10/11	Ann. Bib. Due
10/13	**Fall Break - No Class**
10/18	**Problem Set 2 Due**
10/27	**Mid-Term Exam Due**
11/1	Create and Revise a Slide Due
11/10	Research Grant Proposal "Draft" Due
11/17	Peer Review (Paper) Due
11/22	Practice Presentation & Peer Feedback Due; **Problem Set 3 Due**
11/24	**Thanksgiving Holiday - No Class**
12/1	Final Presentations
12/6	Final Presentations
12/8	Final Presentations; **Problem Set 4 Due**
12/14	**Final Research Grant Proposal Due at 5 pm**

Tips for Success

1. Start early and meet with me to discuss specific resources for your project. In the case you have selected a research project that we will not cover until late in the course, use the recommended readings as a starting point.

2. If you realize after a few weeks that you would like to change research topics or groups, we can do that. Talk to me ASAP about making a change and I will try to accommodate your request.

3. For CHEM 401 students: teamwork is key – you will be wrestling with advanced topics and will benefit from collaboration. For CHEM 501 students or those wishing to pursue a project independently: your peers are still a resource! Develop a cohort to discuss papers, read your work, listen to practice talks, etc.

4. The ability to communicate effectively is critical to your success in the professional world – whether that be as a physician, researcher, teacher, chef, etc. Together we will build and develop your written and oral communication skills. That said, it is your responsibility to make use of writing resources that are available outside of class. I strongly encourage you to make appointments at the WRC. Strunk and White's *The Elements of Style* is an outstanding writing resource (it's also brief, somewhat entertaining, and cheap). A terrific (free) online resource on writing and giving presentations:
https://www.nature.com/scitable/ebooks/englishcommunication-for-scientists-14053993/contents

5. When writing a research paper about advanced topics (some that are new to you) it can be challenging to put ideas from the literature into your own words. If you are concerned about plagiarism, please visit the WRC or talk with me.

6. Some students have reported that the exercise of making and practicing the talk is incredibly useful for paper writing. Consider preparing the talk first (before the paper) to help construct a thoughtful and effective narrative.
7. Easy points: use correct ACS citation format. Format in-text citations using superscript numbers and reference lists appropriately. See:
https://libguides.williams.edu/citing/acs

8. Practice your talk in front of an audience, focusing on transitions between slides. You might consider writing them down. Practice the talk again. And again. When delivering the talk in class it should definitely not be the first time through and it should not be read from note cards, slides, etc. Polished talks that clearly, concisely tell a good story will be the most successful (and earn the most credit).