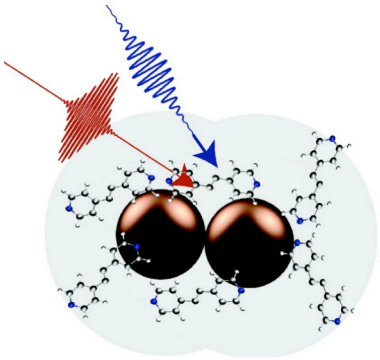
Chem. 401/501: Advanced Physical Chemistry
Spring 2020



Instructor
Prof. Kristin Wustholz, ISC 2041, 1-2675, kwustholz@wm.edu
(email is the best way to contact me)

Class Meetings
TR 2 pm – 3:20 pm, ISC 1111

Office Hours
R 3:30 pm – 4:30 pm (and by appointment**)**

Course Materials
Your physical chemistry and instrumental analysis textbooks may be useful resources for various topics. Other required readings and supplemental resources will be posted on Blackboard.

Course Description
Advanced Physical Chemistry focuses on topics in modern experimental physical chemistry including nanoscience, laser spectroscopy and chemical dynamics, optical and scanning probe microscopy, non-linear optics, and plasmonics. Specific learning goals are to understand fundamentals concepts of light-matter interactions and their applications to current problems in renewable energy, materials science, biology, and atmospheric chemistry. Class meetings will be a mixture of lecture, discussion, in-class exercises, presentation and writing workshops, and student presentations.

Assessment
Research Project Portfolio (40%): A major component of this course involves a semester-long research project where you will become an expert in an active research area in one of the top-20 Ph.D. programs in physical chemistry (*U.S. News & World Report*, 2014). 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, and enhance written and oral communication skills. Chem. 401 students may work in pairs. Chem. 501 students must complete a project individually. Projects will culminate in a research 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 project portfolio that will be turned in at the end of the semester. A complete description of the research project with point breakdown is included on page 4 of this syllabus.

In-Class Exercises and Problem Sets (10%): To help prepare you for exams and research projects, there will be several in-class exercises and a few problem sets (due dates TBD). Collaboration on in-class exercises is encouraged. However, to facilitate the development of independent problem-solving skills, problem sets must be completed individually.

Exams (20% each): Both the mid-term and final are take-home exams. Exams are open note (in-class handouts, exercises, textbooks, and Blackboard materials), but using additional resources (e.g., the internet, other students, publications, etc.) is not permitted. The take-home final exam is due one week after distribution and by the end of the scheduled final exam period: 5 pm on Wednesday, May 13th.

Participation (10%): This course embraces an active learning environment in which your full engagement is vital to the learning experience. Full participation includes coming to class prepared, asking and answering questions, sharing in discussion, collaborating and communicating effectively with your peers, completing in-class exercises, and delivering presentations.

Grades

Grading rubrics for the research project will be posted on Blackboard in advance of the assignment deadline. In general, class scores and grades will be scaled with the following considerations:

A = Excellent performance and mastery of the material
B = Very good understanding of the material
C = Adequate performance
D = Poor performance
F = Unsatisfactory performance

Policies

Late submission of materials is not permitted (except in rare extenuating circumstances). Two class absences for any reason are excused without penalty, but to pass the class, your attendance at the practice and final presentations is mandatory. Additional unexcused class absences will lead to a grade-letter reduction in your participation and/or final grade. Any exceptions to these policies will be at the instructor's discretion in consultation with the Dean of Students Office (757-221-2510, deanofstudents@wm.edu).

Honor Code

The student Honor Code is an important part of what makes W&M a special community. I expect you to observe the Honor Code fully and faithfully.

Class Climate

This course is designed to give you an opportunity to explore topics in advanced physical chemistry through instruction, discussion, and collaboration. Together we will create and maintain an atmosphere of mutual respect in which everyone's ideas can be heard. Please feel free to inform me of the appropriate name and pronoun to use when addressing you.

Writing Resource Center

The Writing Resources Center, located on the first floor of Swem Library, is a free service provided to W&M students. Trained consultants offer individual assistance with writing, presentation, and other communication assignments across disciplines and at any stage, from generating ideas to polishing a final product. Students are encouraged to make use of this free resource. To make an appointment, visit: www.wm.edu/wrc.

Accommodations

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. If you feel that there is anything I can do to ensure a better learning environment for you, please do not hesitate to contact me. As long as these accommodations do not unfairly disadvantage other students, I am more than willing to help out.

Chem 401/501 Tentative Course Schedule:

Week	Topics	Reading	Important Dates
1/20	Welcome & State of the Field: Overview of 401/501 Research Topics	Research project guidelines	
1/27	Light-Matter Interactions, Wave Mechanics, Scattering	Hecht, Ch.2	Add/drop ends 1/31
2/3	Workshop: Research & Citation Tools Absorption, Intro to Perturbation Theory	(McQuarrie, Ch. 6) Levine, 9.1-9.2	2/6: Meet in the Kyle Classroom (Swem)
2/10	Time-Independent and Time-Dependent Perturbation Theory	Levine, 9.9	2/11: *Choose 2 PIs* due
2/17	Fermi's Golden Rule, Resonance, Jablonski Diagram	McQuarrie, 15.1-15.2; Turro, Ch. 5	
2/24	Lasers, Non-Linear Optics	McQuarrie 15.3-15.7	2/27: No class meeting
3/2	Optical and Single-Molecule Microscopy, Single-Photon Counting	*Science* article	3/3*: Ann. Bib.* due 3/6: Deadline for ann. bib. meeting
3/9	*SPRING BREAK*		
3/16	Chemical Dynamics, Transient Absorption Spectroscopy	McQuarrie 15.8	3/19: *Exam 1* due
3/23	Workshop: Presentation Skills; Time-Resolved Vibrational Spectroscopy	Video lecture; *J. Raman Spec.* article	3/24: No class meeting, *Create & Revise a Slide* due
3/30	Nanoscience, Scanning Probe Microscopy	Feynman lecture	*3/31: Paper "Draft"* due
4/6	Nanoparticles, Quantum Dots, Plasmonics, Surface-Enhanced Spectroscopy	*Ann. Rev. Phys. Chem.* article	*4/7: Peer Review (Paper)* due
4/13	Workshop: Practice Presentations & Peer Review	Peer review form	*Practice presentation & peer feedback* due
4/20	Final Presentations		4/30*: Project Portfolio* due
4/27	Final Presentations; Advanced Topic: Class Choice	Journal article TBD	

The **final exam** can be picked up as early as Friday, 4/28 and is due within one week and no later than Wednesday, 5/13 at 5 pm. Pick up time must be scheduled in advance.

Research Project Guidelines

List of Possible Principal Investigators:

Jean-Luc Ayitou (Illinois Tech) – physical organic chemistry, photochemistry
Luis Campos (Columbia) – single-molecule spectroscopy, materials, organic
Fleming Crim (Wisconsin) – reaction dynamics, transient absorption spectroscopy
Jillian Dempsey (UNC) – solar energy, proton coupled electron transfer, inorganic
Gordana Dukovic (Colorado) – quantum dots, nanoscience, ultrafast spectroscopy
Renee Frontiera (Minnesota) – ultrafast spectroscopy, plasmonics, biological sensing
Daniel Gamelin (Washington) – inorganic, luminescence, plasmonics, quantum dots
Naomi Ginsburg (UC Berkeley) – single-molecule spectroscopy, organic photovoltaics
Naomi Halas (Rice University) – plasmonics, nanoscience, catalysis
Marsha Lester (UPenn) – atmospheric chemistry, vibrational spectroscopy
Amanda Morris (Virginia Tech) – spectroscopy, catalysis, metal organic frameworks
Cathy Murphy (Illinois) – nanoscience, inorganic, nanomedicine, plasmonics
Eric Potma (UC Irvine) – nonlinear microscopy, tissue imaging
Ben Schwartz (UCLA) – resonance Raman, ultrafast spectroscopy, hydrated electron
Gregory Scholes (Princeton) - solar energy conversion, ultrafast spectroscopy
Claudia Turro (Ohio State) - ultrafast spectroscopy, inorganic complexes, photodynamic therapy
Haw Yang (Princeton) – protein dynamics, quantum dots, single-molecule spectroscopy

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 paper and presentation. You will learn how to use reference management software and cite in ACS format. (*Kyle Classroom, Swem Library on Thursday, 2/6*)

2. *Choose 2 PIs (~1 page):* Investigate the PIs listed above (**and others if you wish**). Find publications on their website and Web of Science 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 Tuesday, 2/11*)

3. *Annotated Bibliography (~5 pages):* Once PI assignments are finalized, you will have 2.5 weeks to pursue an in-depth study of the 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 in class on Tuesday, 3/3*) Each individual/team will meet with the instructor outside of class to discuss the sources, annotated bibliography, and recommended revisions. (*No later than Friday, 3/6 at 3 pm*)

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 on Tuesday, 3/24 - no class meeting this day*) Time permitting: your peers will evaluate the revised slide in class.

5. *Research Paper "Draft":* Submit two copies of a "draft" of the 7-8 page (not including references) research paper. 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 Tuesday, 3/31*)

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 Tuesday, 4/7*)

7. *Workshop: 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 the week of 4/13*)

8. *Class Presentation and Discussion:* Present a 20-min. 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 Tuesday, 4/21 and Thursday, 4/30*)

9. *Project Portfolio:* Submit the complete research project 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 paper, 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 Thursday, 4/30*)

Points Breakdown:

1. Choose Two PIs (10 pts)
2. Annotated Bibliography (30 pts)
3. Create & Revise a Slide (15 pts)
4. Research Paper "Draft" (30 pts)
5. Peer Review a Paper (15 pts)
6. Practice Presentations & Peer Feedback (30 pts)
7. Class Presentations and Discussion (50 pts)
8. Response to Reviewers (10 pts)
9. Final Research Paper (50 pts)
10. Self/Group Evaluation (10 pts)
    Total = 250 pts (40% of final grade)

Tips for Success from Previous Students:

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/english-communication-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).