Course Syllabus – CHEM 421

Course Information

Course Number: CHEM 421 SP24
Course Name: Computational and Analytical Tools for Chemists
Term: Spring 2024
Start Date: 04/01/2024
End Date: 06/21/2024
Credits: 3.0

Meeting Days / Times

Mondays and Wednesdays, 9:00-10:30am PT / 12:00-1:30pm ET
(See Calendar in Canvas for the most up-to-date schedule.)

Location

CA: Keck Amphitheater (except April 29 - Grad Office Seminar Room)
FL: B214

Course Managers

Role	Last Name	First Name	Email Address
Course Director	Engle	Keary	keary@scripps.edu
TA	Li	Chunyu	chli@scripps.edu

Course Description

This class provides students with a foundation in computational and analytical techniques that undergird modern research in the chemical sciences. Covered topics include density functional theory, nuclear magnetic resonance spectroscopy, mass spectrometry, and X-ray crystallography.

Program Learning Outcomes

By the end of the program, students will have accomplished these objectives:
PLO1: Original Research – graduate students are expected to develop the skills critical for generating high-quality research output. This would include absorbing, recalling, and contextualizing scientific knowledge, evaluating scientific information and data, creating testable hypotheses and investigating hypotheses, mastering scientific tools and techniques, displaying ethical behavior, and receiving and giving feedback.

PLO2: Communication – graduate students are expected to demonstrate the oral, written, and media skills to effectively communicate the impact of a study or a body of work to the greater scientific community and to the public at large using a number of methods.
PLO3: Critical Thinking – graduate students are expected to develop a self-directed process to analyze information, form opinions or judgments, and use this process to improve the quality of their scientific thoughts, navigate problems, and make informed decisions.
PLO4: Intellectual Curiosity – graduate students are expected to acquire the capacity to build their intellectual curiosity and demonstrate problem solving approaches that serve their professional growth and ability to impact a field.
PLO5: Career and Professional Development – graduate students are expected to develop a variety of transferable skillsets throughout their graduate experience, including management and leadership, inclusiveness, resilience, scientific rigor, collaboration, accountability, time management, teamwork, networking, and career planning.

For a detailed description of each outcome and specific success indicators, please refer to this web page: https://education.scripps.edu/graduate/doctoral-program/.

Course Learning Outcomes

By the end of this course, students will be able to:
CLO1: Select an appropriate analytical technique to ask and answer research questions in chemistry.
CLO2: Understand the underlying theory behind commonly used analytical and computational methods.
CLO3: Read academic literature and understand how data collected from the techniques covered is used to support conclusions drawn

Background Preparation (Prerequisites)

N/A

Course Materials

Required: Silverstein, Webster, Kiemle & Bryce. *Spectrometric Identification of Organic Compounds* (8th Edition). ISBN: 978-0470616376
Useful to consult: Berger & Braun. *200 and More Basic NMR Experiments: A Practical Course* (1st Edition). ISBN: 978-3527310678
Useful to consult: Sanders & Hunter. *Modern NMR Spectroscopy: A Guide for Chemists* (2nd Edition). ISBN: 978-0198555674
Useful to consult: Derome. *Modern NMR Techniques for Chemistry Research* (Reprint). ISBN: 978-0080325132
Useful to consult: Siuzdak. *The Expanding Role of Mass Spectrometry in Biotechnology* (2nd Edition). ISBN: 978-0974245126

Useful to consult: Claridge. *High-Resolution NMR Techniques in Organic Chemistry* (3rd Edition). ISBN: 978-0080999869

Expectations and Logistics

Students are expected to attend all scheduled classes, participate in class-related activities, and complete problem sets and projects on time.

Class Format

This class will consist of two interactive lectures per week. In-class learning will be supplemented with take-home problems sets and projects.

Attendance Statement

Students are expected to attend all classes. Students who are unable to attend class must seek permission for an excused absence from the course director or teaching assistant. Unapproved absences or late attendance for three or more classes may result in a lower grade or an "incomplete" for the course. If a student has to miss a class, he or she should arrange to get notes from a fellow student and is strongly encouraged to meet with the teaching assistant to obtain the missed material.

Scientific and Professional Ethics

The work you do in this course must be your own. Feel free to build on, react to, criticize, and analyze the ideas of others but, when you do, make it known whose ideas you are working with. You must explicitly acknowledge when your work builds on someone else's ideas, including ideas of classmates, professors, and authors you read. If you ever have questions about drawing the line between others' work and your own, ask the course professor who will give you clear guidance. Exams must be completed independently. Any collaboration on answers to exams, unless expressly permitted, may result in an automatic failing grade and possible expulsion from the Graduate Program.

Technology Requirements and Support

For issues related to Canvas, please contact the Graduate Office by email at: gradprgm@scripps.edu or by phone at: 858-784-8469.

Course Grading

Grading is in accordance with the academic policies of the Skaggs Graduate School. The breakdown of grading is as follows:

- Attendance and Participation: 10%
- NMP Problem Set: 10%
- DFT Midterm Project: 40%
- Final Project: 40%

Grade Point	Letter Grade	
4.00	A	Outstanding achievement. Student performance demonstrates full command of the course subject matter and evinces a high level of originality and/or creativity that far surpasses course expectations.
3.67	A-	Excellent achievement. Student performance demonstrates thorough knowledge of the course subject matter and exceeds course expectations by completing all requirements in a superior manner.
3.33	B+	Very good work. Student performance demonstrates above-average comprehension of the course subject matter and exceeds course expectations on all tasks as defined in the course syllabus. There is notable insight and originality.
3.00	B	Satisfactory work. Student performance meets designated course expectations and demonstrates understanding of the course subject matter at an acceptable level.
2.67	B-	Marginal work. Student performance demonstrates incomplete understanding of course subject matter. There is limited perception and originality.
2.33	C+	Unsatisfactory work. Student performance demonstrates incomplete and inadequate understanding of course subject matter. There is severely limited or no perception or originality. Course will not count toward degree.
2.00	C	Unsatisfactory work. Student performance demonstrates incomplete and inadequate understanding of course subject matter. There is severely limited or no perception or originality. Course will not count toward degree.
0.00	I	Incomplete is assigned when work is of passing quality but is incomplete for a pre-approved reason. Once an incomplete grade is assigned, it remains on student's permanent record until a grade is awarded.

0.00	P	Satisfactory work. Student performance demonstrated complete and adequate understanding of course subject matter. Course will count toward degree.
0.00	F	Unacceptable work/Failure. Student performance is unacceptably low level of knowledge and understanding of course subject matter. Course will not count toward degree. Student may continue in program only with permission of the Dean.
0.00	W	Withdrew from the course with Dean's permission beyond the second week of the term.

- All courses will be recorded and maintained in the student's permanent academic record; only courses that apply towards the degree will appear on the academic transcript. Non-credit or audited courses will not appear on the transcript.
- 4 core courses taken for a letter grade (pass = B- or higher for a core course)
- 2 elective courses taken pass/fail (pass = A, B, C for an elective)

Course Summary

Date	Details
Mon Apr 1, 2024	DFT (Karunananda + Houk)
Wed Apr 3, 2024	DFT (Karunananda + Houk)
Mon Apr 8, 2024	DFT (Karunananda + Houk)
Wed Apr 10, 2024	DFT (Karunananda + Houk)
Mon Apr 15, 2024	DFT (Karunananda + Houk)
Wed Apr 17, 2024	DFT (Karunananda + Houk)
Mon Apr 22, 2024	NMR (Huang + Pasternack)
Wed Apr 24, 2024	NMR (Huang + Pasternack)
Mon Apr 29, 2024	NMR (Huang + Pasternack)
Wed May 1, 2024	NMR (Huang + Pasternack)
Mon May 6, 2024	NMR (Huang + Pasternack)
Wed May 8, 2024	NMR Advanced Problems (Köck)
Mon May 13, 2024	NMR Advanced Problems (Köck)
Wed May 15, 2024	NMR Advanced Problems (Köck)
Fri May 17, 2024	Commencement
Mon May 20, 2024	X-ray (Gembicky)
Wed May 22, 2024	X-ray (Gembicky)
Mon May 27, 2024	No Class (Memorial Day)
Wed May 29, 2024	Mass Spec (Chen)

Mon Jun 3, 2024	Mass Spec (Chen)
Wed Jun 5, 2024	micro-ED (Nelson)
Mon Jun 10, 2024	Absorption and Fluorescence (Zimmerman
Wed Jun 12, 2024	Absorption and Fluorescence (Zimmerman)
Mon Jun 17, 2024	Final Project Presentations
Wed Jun 19, 2024	No Class (Juneteenth)