Term Information

Effective Term	Spring 2023
Previous Value	*Summer 2012*

Course Change Information

What change is being proposed? (If more than one, what changes are being proposed?)

Request to change the CHEM 7470 course to a 14-week offering and a 2-credit hour course.

What is the rationale for the proposed change(s)?

Full course history and rationale is included in the attachment "Rationale for CHEM 7470 changes". Briefly, there would be no changes in the learning goals or course outcomes. The change to a 14-week course offering is being requested to allow efficient completion of the student project, while avoiding the process of assigning an incomplete grade to each student. The change from 1.5 to 2 credit hours is to account for the additional office hours and hands-on assistance from the instructor and TA during the additional 7-weeks of the course.

What are the programmatic implications of the proposed change(s)?

(e.g. program requirements to be added or removed, changes to be made in available resources, effect on other programs that use the course)?

This course is an optional elective so the change from 1.5 to 2.0 would have no effect on any major. As an example, even in Chemistry and Biochemistry, graduate students are often required to take at least 3.0 credits of 7000-level courses, and this change would have no meaningful impact on our graduate students as two 1.5-credit hour courses, or a combination of a 1.5- and a 2.0-credit courses would be needed.

Is approval of the requrest contingent upon the approval of other course or curricular program request? No

Is this a request to withdraw the course? No

General Information

Course Bulletin Listing/Subject Area	Chemistry
Fiscal Unit/Academic Org	Chemistry - D0628
College/Academic Group	Arts and Sciences
Level/Career	Graduate
Course Number/Catalog	7470
Course Title	Computational Chemistry
Transcript Abbreviation	Computational Chem
Course Description	A practical and theoretical treatment of advanced computational chemistry, from molecular mechanics to electronic structure methods and with an examination of the application of computational methods for providing guidance to experimental studies.
Semester Credit Hours/Units	Fixed: 2
Previous Value	*Fixed: 1.5*

Offering Information

Length Of Course	14 Week, 8 Week, 7 Week, 6 Week
Previous Value	*8 Week, 7 Week, 6 Week*
Flexibly Scheduled Course	Never
Does any section of this course have a distance education component?	No
Grading Basis	Letter Grade
Repeatable	No

Course Components	Lecture
Grade Roster Component	Lecture
Credit Available by Exam	No
Admission Condition Course	No
Off Campus	Never
Campus of Offering	Columbus

Prerequisites and Exclusions

Prerequisites/Corequisites	Prereq: Permission of instructor.
Exclusions	
Previous Value	Not open to students with credit for 944.
Electronically Enforced	No

Cross-Listings

Cross-Listings

Subject/CIP Code

Subject/CIP Code	40.0504
Subsidy Level	Doctoral Course
Intended Rank	Junior, Senior, Masters, Doctoral

Requirement/Elective Designation

The course is an elective (for this or other units) or is a service course for other units

Course Details

Course goals or learning objectives/outcomes

- Provide a practical introduction to the theory and mechanics of computational chem, especially for its use by experimentalists; hands-on practice in doing molecular mechanics, semi-empirical, ab initio quantum chem & density functional theory

Previous Value

Content Topic List

- Computational chemistry
- Molecular mechanics
- Electronic structure theory
- Molecular dynamics
- Molecular docking
- Calculating excited states
- Vibrational properties
- NMR properties
- Chiroptical properties
- Theoretical chemistry
- Calculations

Sought Concurrence No

Attachments

- Chem_7470_Syllabus_Sp2022.docx: Current syllabus

  (Syllabus. Owner: Hambach,Jennifer Lynn)

- Proposed_New_Chem_7470_Syllabus.docx: New syllabus

  (Syllabus. Owner: Hambach,Jennifer Lynn)

- Rationale for CHEM 7470 Changes.docx: Rationale

  (Other Supporting Documentation. Owner: Hambach,Jennifer Lynn)

Comments

Workflow Information

Status	User(s)	Date/Time	Step
Submitted	Hambach,Jennifer Lynn	04/19/2022 10:43 AM	Submitted for Approval
Approved	Wade,Christine M.T	04/19/2022 11:42 AM	Unit Approval
Approved	Vankeerbergen,Bernadette Chantal	05/02/2022 11:51 AM	College Approval
Pending Approval	Cody,Emily Kathryn Jenkins,Mary Ellen Bigler Hanlin,Deborah Kay Hilty,Michael Vankeerbergen,Bernadette Chantal Steele,Rachel Lea	05/02/2022 11:51 AM	ASCCAO Approval

Christopher M. Hadad hadad.1@osu.edu

Chemistry 7470 Spring 2023

Lecture: Monday/Wednesday/Friday 3:00 – 3:55 pm 2001 Evans Lab
The class will have lecture for approximately the first 7-8 weeks of the 14-week term, followed by your final exam around the 8th week, and then the remaining 7 weeks of the term will be dedicated to your computational chemistry project, along with technical support from your teaching assistant and myself.

Instructor: Professor Christopher M. Hadad
183 CBEC (614) 688–3141 hadad.1@osu.edu
Office Hours: Stop by anytime (and often). E-mail as needed. Or call.

All students with disabilities who need accommodations should see me privately to make arrangements.

TA: Yiran (Amy) He (he.1768@osu.edu, 410 CBEC, with additional office hours for 0008 McPherson Lab and OSC usage)

Textbook: *Essentials of Computational Chemistry: Theories and Models* by Christopher J. Cramer

Other reference materials are available:

Introduction to Computational Chemistry by Frank Jensen
Ab Initio Molecular Orbital Theory by Warren Hehre, Leo Radom, Paul v. Rague Schleyer and John Pople
Molecular Mechanics by Ulrich Burkert and Norman Allinger
Computational Chemistry by G. H. Grant and W. G. Richards
Encyclopedia of Computational Chemistry, Schleyer, P. v. R., Ed. (Volumes 1 –5)
Modelling Molecular Structures by Alan Hinchliffe

Prerequisites: Completion (or near completion) of first-year graduate courses at Ohio State.

Objectives: To provide a *practical* introduction to the theory and mechanics of computational chemistry, especially for its use by experimentalists. Hands-on practice will be obtained by all attendees in doing molecular mechanics, semi-empirical, *ab initio* quantum chemistry and density functional theory. As time permits, we will explore molecular dynamics, ligand docking into active sites, and other topics.

Software: All students will be provided access to molecular modeling software (Gaussian, Spartan, Chem3D, MOE/Yasara, TurboMole and MacroModel) in order to practice with computational chemistry and biochemistry. The software will be available on the computers in the department as well as the Ohio Supercomputer Center (OSC).

Visualization will occur on the Macs and PCs in the department – we will provide details on how to do that. The software will be made available by the department of Chemistry and Biochemistry and by the OSC. We will arrange access to these resources for you – via the official roster.

We have some visualization software on the Macs and PCs in the lab, and if you have a personal computer, you can let me know. We have appropriate licenses for certain hardware.

Grades: Your final grade will be determined by your performance on the **problem sets (40%)**, on the **"research project" (30%)**, on the **final exam (30%)**.

There will only be one exam for the course, and we can discuss the possible date and time:

Exam Soon after End of first 7-week term Time and Location TBD

Problem sets (40%) will be handed out in class, and will be due when specified – you will usually have one week to perform the problem set. There will be approximately 6 problem sets for the entire course.

For the problem sets, you MUST do all of the work yourself. You are welcome to collaborate with your colleagues and to discuss how to do the calculations. **However, you must do all of the calculations individually and submit a written report so that it is clear that you have done the work yourself.** If we have any doubts, we will ask for verification that you have done the individual calculations for each and every problem set. Obviously, it would be useful to you to keep your files for each problem set separately (perhaps as a directory or folder with your data files).

Any concerns about academic misconduct will be reported to the Committee on Academic Misconduct for their adjudication.

This course is meant to be a practical introduction, so besides attending lectures, each student will be expected to work on a "major" computational project – as suggested by the student. If you have difficulty coming up with a topic, please discuss the matter with me.

You will be asked around the 5th week of the term to submit an abstract of the topic of your project/paper. You can consult with your research advisor (and us) about possible ideas, both for value and for practical completion during the semester. It is hoped that each student will pursue a research idea that is of interest to them and then try to apply a computational approach to assist in its revelation.

A report (15 – 20 pages, double spaced, including tables and figures) on this project should be written in the style of an article to the *Journal of the American Chemical Society* or similar ACS journal, complete with abstract, introduction, methods, results, tables, figures, conclusions and references.

The due date for your project/paper will be Monday, April 25, 2022 by 11 pm ~~– thus, each of you will get an "incomplete" for the first-half term and then your final grade will be determined after your final report is delivered (and graded).~~ You are welcome to turn in the report earlier, if that is convenient to your summer research plan.

Your scores will be listed on Carmen at:

https://carmen.osu.edu

Dates: Please see the URL: https://registrar.osu.edu/registration for important registration and withdrawal dates.

Christopher M. Hadad hadad.1@osu.edu

Chemistry 7470 Spring 2022

Lecture: Monday/Wednesday/Friday 3:00 – 3:55 pm 2001 Evans Lab

Instructor: Professor Christopher M. Hadad
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Office Hours: Stop by anytime (and often). E-mail as needed. Or call.

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We have some visualization software on the Macs and PCs in the lab, and if you have a personal computer, you can let me know. We have appropriate licenses for certain hardware.

Grades: Your final grade will be determined by your performance on the **problem sets (40%)**, on the **"research project" (30%)**, on the **final exam (30%)**.

There will only be one exam for the course, and we can discuss the possible date and time:

Exam Saturday, February 26, 2022 (?) Time TBD Location TBD

Problem sets (40%) will be handed out in class, and will be due when specified – you will usually have one week to perform the problem set. There will be approximately 6 problem sets for the entire course.

For the problem sets, you MUST do all of the work yourself. You are welcome to collaborate with your colleagues and to discuss how to do the calculations. **However, you must do all of the calculations individually and submit a written report so that it is clear that you have done the work yourself.** If we have any doubts, we will ask for verification that you have done the individual calculations for each and every problem set. Obviously, it would be useful to you to keep your files for each problem set separately (perhaps as a directory or folder with your data files).

Any concerns about academic misconduct will be reported to the Committee on Academic Misconduct for their adjudication.

This course is meant to be a practical introduction, so besides attending lectures, each student will be expected to work on a "major" computational project – as suggested by the student. If you have difficulty coming up with a topic, please discuss the matter with me.

You will be asked around the 5th week of the term to submit an abstract of the topic of your project/paper. You can consult with your research advisor (and us) about possible ideas, both for value and for practical completion during the semester. It is hoped that each student will pursue a research idea that is of interest to them and then try to apply a computational approach to assist in its revelation.

A report (15 – 20 pages, double spaced, including tables and figures) on this project should be written in the style of an article to the *Journal of the American Chemical Society* or similar ACS journal, complete with abstract, introduction, methods, results, tables, figures, conclusions and references.

The due date for your project/paper will be Monday, April 25, 2022 by 11 pm – thus, each of you will get an "incomplete" for the first-half term and then your final grade will be determined after your final report is delivered (and graded). You are welcome to turn in the report earlier, if that is convenient to your summer research plan.

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Dates: Please see the URL: https://registrar.osu.edu/registration
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CHEM 7470 Computational Chemistry

Request to change the CHEM 7470 course to a 14-week offering and a 2-credit hour course.

First, a brief synopsis and history of the current course. This graduate-level Computational Chemistry course has always incorporated a student-selected project as part of the grade. When the course was created under quarters (then, CHEM 944), the course used the 10-week quarter to provide lectures, along with assigned problem sets and a final exam, and most importantly, the student-selected project in conjunction with the student's advisor. This project allowed the student to apply the computational methods of interest to a problem, usually an experimental problem, of particular interest to that specific research group.

And, I should add that since this course began, about 40 of those projects have been published by the student and their advisor as I have always helped the student/advisor to continue the work, either providing a computational aspect to the PhD student's thesis or peer-reviewed publications.

Under quarters, the students would decide their project in the 4th or 5th week of the quarter, and then would have to rush to finish the project by the 10th week of the term.

When this course was converted to semesters, it was converted to a 1.5 credit hour, 7-week offering, and there was not sufficient time to learn enough about the various computational methods, decide the focus of the project and then also complete and write up the results of the project in 7 weeks. So, since semester conversion, we have functioned in this manner:

- Students select their project in the 4th week of the term, submitting an abstract to ensure practicality.
- After the 7 weeks of lecture content and problem sets, the students have a final exam around the 8th week.
- Each student is given an incomplete grade by the end of the 7th week, allowing them to work on their project until the end of the 14-week semester.
- After submission of their final project report, the incomplete is changed to the final grade.

What we are currently requesting is the following.

- There would be no changes in the learning goals or course outcomes. This change is being requested to allow efficient completion of the student project, while avoiding the process of assigning an incomplete grade to each student.
- I would like to change the course to a 14-week offering, but in-person lecturing will occur for the first 7 weeks of the term.
- The students would work on typical problem sets for the first 7 weeks of the term.
- The students would finish their "final exam" in the 8th or 9th week of the term, depending on the most convenient schedule for the students.
- Students would still select their project's topic in the 4th week of the term.
- Students would then have until the end of the 14-week term to submit their project report for final grading.
- This new process would remove the need for any incomplete grades.

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- During the remaining 7 weeks of the 14-week term, the assigned teaching assistant (TA) and I will continue to have office hours for hands-on assistance, including implementing a regularly scheduled set of office hours in the computer lab for the assigned TA.
- With the additional office hours and hands-on assistance, we request changing the class to 2 credit hours, from the current 1.5 credit hours. This course is an optional elective so the change from 1.5 to 2.0 would have no effect on any major. As an example, even in Chemistry and Biochemistry, graduate students are often required to take at least 3.0 credits of 7000-level courses, and this change would have no meaningful impact on our graduate students as two 1.5-credit hour courses, or a combination of a 1.5- and a 2.0-credit courses would be needed.