

Class Syllabus Template

(1) Course Number: CH412/612

(2) Course Title: Computational Chemistry

(3) Catalog Description: Applications of theoretical chemistry including molecular modelling and quantum mechanical calculations in the high performance computing environment.

(4) Prerequisites: CH312

(5) Co-requisites: CS101

(6) Credit Hours: 3.0

(7) Semester: Fall only

(8) Class Meeting Time(s), location and format: 3 lecture hours per week

(9) Instructor: [Dr. Marcus Bond

(10) Instructor Contact Information: mbond@semo.edu, 651-2580, RH230A]

(11) Concerns: Questions, comments or request regarding this course should be taken to the instructor. Unanswered questions or unresolved issues about this class can be directed to Dr. Philip Crawford, Chairperson, Department of Chemistry & Physics.

(12) Course Learning Outcomes:

1. Students will be able to demonstrate an understanding of the theoretical foundations of computational molecular and quantum mechanics.
2. Students will be able to perform computational studies of molecular systems using molecular and quantum mechanics.
3. Students will be able to demonstrate an ability to compile software and launch computational from both the command line and user gateways in a POSIX high computing environment.

(13) Course-specific Required Materials:

Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics 3rd ed. Frank W. Lewars

(14) Course Content:

Week 1: Fundamentals of Quantum Chemistry (review)

Week 2- Overview of Computational Chemistry and the Potential Energy Surface

Week 3: Molecular Mechanics

Week 4: Simple Huckel based Molecular Orbital Theory and Calculations

Week 5-6: Semi-empirical Molecular Orbital Calculations

Weeks 7-9: *ab initio* Molecular Orbital Calculations

Weeks 10-11: Density Functional Calculations

Week 12-13: Computational Chemistry in the High Performance Computing Environment

Week 14-15: Special Advanced Topics

There will be three one-hour exams at the 5th, 10th and 15th week worth 15% each of the total grade. A comprehensive two hour final exam worth 30% of the grade will be offered at the time specified in the University Final Exam schedule. Homework both paper and computer exercises, will be assigned each week and worth 25% of the CH412 grade and 15% of the CH612 grade. Students in CH612 will complete an independent study module on molecular dynamics that will constitute 10% of the grade in CH612

(15) Grading Scale and Policies:

Undergraduate: Grades will be assigned using the standard grading scale of:

- A, ≥90% of the total grade
- B, ≥80% of the total grade
- C, ≥70% of the total grade
- D, ≥60% of the total grade
- F, <60% of the total grade

Graduate: Grades will be assigned using the standard grading scale of:

- A, ≥90% of the total grade
- B, ≥80% of the total grade
- C, ≥70% of the total grade
- F, <60% of the total grade

Exams are to be taken on the assigned day unless prior arrangements are made. Homework is due one week after it is assigned. Due to the need for students to stay current with the class material, late homework or extensions on homework will not be permitted.

(16) Final Exam Schedule: According to the University schedule.

(17) A laptop computer is recommended but not required.

(18) **Academic Honesty** – Southeast Missouri State University expects all students, faculty and staff to operate in an honest and ethical manner. Academic dishonesty is a very serious offense because it undermines the value of your education and the education of others. Students who engage in academic dishonesty face significant penalties. Forms of academic dishonesty include, but are not limited to, plagiarism, cheating, contract cheating, misrepresentation, and other actions you take. Some of these are defined below:

- Plagiarism means passing off someone else's work as your own, whether it is intentional or unintentional.
- Cheating includes copying from another person or source of information to meet the requirements of a task.
- Contract cheating is paying someone else or a company to do your work.
- Misrepresentation means you are posing as someone else or someone else is posing as you to complete a task.
- Collusion means working with one or more people to cheat. If you help someone cheat or plagiarize you will face the same penalties.

For more information, visit the Responsible Redhawks Code of Conduct <http://www.semo.edu/responsibleredhawks/code-of-conduct.html> or the Faculty Handbook Section (D) on Academic Honesty <http://www.semo.edu/facultysenate/handbook/5d.html>

(19) **Accessibility** – Southeast Missouri State University and Disability Services are committed to making every reasonable educational accommodation for students who identify as people with disabilities. Many services and accommodations which aid a student’s educational experience are available for students with various disabilities. Students are responsible for contacting Disability Services to register and access accommodations. Accommodations are implemented on a case by case basis. For more information, visit <http://www.semo.edu/ds/> or contact Disability Services at 573-651-5927.

(20) **Civility** – Your university experience is purposely designed to introduce you to new ideas, help you think effectively, develop good communication skills, evaluate information successfully, distinguish among values and make sound judgements. Doing this well requires respectful and courteous discussion among and between students and the instructor. Together, we must create a space where we acknowledge and respect others have different experiences, perspectives and points of view. Disagreements are likely. Mutual respect for one another and a willingness to listen are important. Remember, you are responsible for your behavior and actions. There is a no tolerance policy on bullying or harassment of any kind. Additional information on student conduct may be found at: <http://www.semo.edu/pdf/stuconduct-code-conduct.pdf?ver=1.0> and http://www.semo.edu/pdf/Conduct_Faculty_Resource_Guide.pdf

(21) **Mandatory Reporting** – I will keep information you share with me confidential to the best of my ability, but as a professor I am legally required to share information about sexual misconduct and crimes I learn about to make our campus and community safe for everyone.

(22) **Student Success** – This course uses SupportNET, Southeast’s student success network, to improve communication between students, faculty and staff on campus. You’ll get emails through SupportNET with information about resources or concerns. Please read these emails—they are sent to help you succeed! You can access SupportNET through your portal, Moodle or directly at supportnet.semo.edu to see any academic alerts, ask for help and to access resources to support your success at Southeast.

*Definition of ‘blended’ to be added.

COURSE APPROVAL/CHANGE DOCUMENT

(See back of form for instructions)

Submit

1. ADDITION REVISION TERMINATION

2. IF REVISION: denote changes (i.e. Title only; Title, CIP and Description, etc.):

3. COURSE NUMBER CH 412

4. COURSE TITLE Computational Chemistry

5. IF REVISION: Previous Course No. _____ Previous Title _____

6. FOR ADDITIONS AND REVISIONS -
FIRST TERM/YEAR TO BE OFFERED:

Fall Spring Summer Term 2020

7. FOR TERMINATIONS ONLY -
LAST TERM/YEAR TO BE OFFERED:

Fall Spring Summer Term _____

8. COLLEGE: Coll of Sci, Tech, Engr & Math

9. DEPARTMENT NAME: Chemistry & Physics

10. CIP CODE (Classification of Instructional Program / US Bureau of Labor Statistics): 40.0501

11. FIXED CREDIT HOURS: YES NO

3 Total Credit Hours

3 Lec Contact Hours

___ Lab Contact Hours

___ Other Contact Hours

12. VARIABLE CREDIT HOURS: YES NO

___ Min Total Credit Hours ___ Max Total Credit Hours

___ Min Lec Contact Hours ___ Max Lec Contact Hours

___ Min Lab Contact Hours ___ Max Lab Contact Hours

___ Min Other Contact Hours ___ Max Other Contact Hours

13. CAN THIS COURSE BE TAKEN FOR ADDITIONAL CREDIT: YES NO If YES, total number of times course can be taken _____

14. MAXIMUM ENROLLMENT ALLOWED FOR COURSE: 12 Justification of maximum enrollment:

This class requires Advanced Physical Chemistry as a prerequisite. This class has an enrollment limit of 12 due to the advanced nature of the material and the resulting need for a high degree of student-teacher interaction. This class is even more advanced, and requires the same enrollment limit.

15. CLASS SCHEDULE TYPE/ FACULTY WORKLOAD: Choose appropriate schedule type: L - Lecture

Faculty Workload: 3.0 Class schedule type justification:

This is a renumbered version of a class that has previously been taught as CH663, Topics in Inorganic Chemistry. This was a 3 credit hour class with 2 lecture hours and two lab hours. It was taught at a lower level, justifying fewer lecture hours, and at the time the chemistry department laptops were needed for some activities, which required the lab. CH412 will be taught at a higher level, hence requiring more lecture time, while all exercise are available through student's personal devices or university computer labs, thus making a lab period unnecessary.

16. COURSE LEVEL: Undergraduate

17. GRADE TYPE: Standard Grade

18. DEVELOPMENTAL COURSE: YES NO

19. CROSS-LISTED COURSE:

YES WITH _____ NO

20. SPECIAL COURSE FEE? (Must be Board approved)

YES Amount \$ _____ NO

21. Required faculty qualifications to teach this course:

Ph.D in Chemistry with a specialization in Physical Chemistry or Chemical Physics and experience with computation.

22. UNIVERSITY STUDIES COURSE: YES NO

If yes, please select one general education category:

If yes, please select up to three general education learning goals that reflect the priorities for student learning in the course. Please rank these in priority order, i.e. 1,2,3 by inserting the numbers/rankings into the boxes:

- ___ General Education Learning Goal 1: Ethical Reasoning
- ___ General Education Learning Goal 2: Global Learning
- ___ General Education Learning Goal 3: Information Literacy
- ___ General Education Learning Goal 4: Written Communication
- ___ General Education Learning Goal 5: Oral Communication
- ___ General Education Learning Goal 6: Critical Thinking
- ___ General Education Learning Goal 7: Quantitative Literacy

If the proposed new or revised course is a General Education/University Studies course, please provide a short rationale why this course should be considered as a general education course.

Attach the following:

- a) If applicable, memos from Department Chair(s) in affected department(s) stating support or that issues/conflicts are resolved.
- b) Memo from Library Dean assessing available and needed library resources and services.
- c) Class syllabus using the syllabus template: [Syllabus Template Link](#)

COURSE APPROVAL SIGNATURES

Department Chairperson	Dean of Kent Library	College Council
Philip W. Crawford <small>Digitally signed by Philip W. Crawford Date: 2019.04.04 15:15:10 -05'00'</small>	Barbara C. Glackin <small>Digitally signed by Barbara C. Glackin Date: 2019.05.10 11:37:20 -05'00'</small>	Brad Deken <small>Digitally signed by Brad Deken Date: 2019.05.15 08:02:28 -05'00'</small>
Educator Preparation Committee	University Studies Council	Graduate Council

To obtain the next signature, save the pdf to your desktop and then email the form as an attachment to the next individual for signing. When submitting the form, the email must come from your Southeast email account.

Registrar's Office Use Only			
SCACRSE _____	Bulletin _____	Degree Audit _____	SHATATR _____

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1. ADDITION REVISION TERMINATION

2. IF REVISION: denote changes (i.e. Title only; Title, CIP and Description, etc.):

3. COURSE NUMBER CH 612 4. COURSE TITLE Computational Chemistry

5. IF REVISION: Previous Course No. _____ Previous Title _____

6. FOR ADDITIONS AND REVISIONS -
FIRST TERM/YEAR TO BE OFFERED:

Fall Spring Summer Term 2020

7. FOR TERMINATIONS ONLY -
LAST TERM/YEAR TO BE OFFERED:

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____ Min Lec Contact Hours ____ Max Lec Contact Hours

____ Min Lab Contact Hours ____ Max Lab Contact Hours

____ Min Other Contact Hours ____ Max Other Contact Hours

13. CAN THIS COURSE BE TAKEN FOR ADDITIONAL CREDIT: YES NO If YES, total number of times course can be taken _____

14. MAXIMUM ENROLLMENT ALLOWED FOR COURSE: 4 Justification of maximum enrollment:

This class is cross listed with CH412 which has an enrollment limit of 12 to match the limit of the prerequisite class, CH312. The enrollment limit of 4 for the graduate class accounts for the additional work and instruction the graduate students must participate in to justify this as a graduate level class.

15. CLASS SCHEDULE TYPE/ FACULTY WORKLOAD: Choose appropriate schedule type: L - Lecture

Faculty Workload: 3.0 Class schedule type justification:

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16. COURSE LEVEL: Graduate

17. GRADE TYPE: Standard Grade

18. DEVELOPMENTAL COURSE: YES NO

19. CROSS-LISTED COURSE:

YES WITH _____ NO

20. SPECIAL COURSE FEE? (Must be Board approved)

YES Amount \$ _____ NO

21. Required faculty qualifications to teach this course:

Ph.D in Chemistry with a specialization in Physical Chemistry or Chemical Physics and experience with computation. Graduate faculty status.

22. UNIVERSITY STUDIES COURSE: YES NO

If yes, please select one general education category:

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Educator Preparation Committee	University Studies Council	Graduate Council
		Doug Koch <small>Digitally signed by Doug Koch Date: 2019.09.25 14:24:31 -05'00'</small>

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SCACRSE _____	Bulletin _____	Degree Audit _____	SHATATR _____