The Ohio State University
Colleges of the Arts and Sciences New Course Request

Chemistry
Academic Unit
Chemistry
Book 3 Listing (e.g., Portuguese)
644 Computational Chemistry
Number Title
Computational Chem U 3
18-Character Title Abbreviation Level Credit Hours

Summer Autumn X Winter Spring Year 2008
Proposed effective date, choose one quarter and put an "X" after it; and fill in the year. See the OAA curriculum manual for deadlines.

A. Course Offerings Bulletin Information

Follow the instructions in the OAA curriculum manual. If this is a course with decimal subdivisions, then use one New Course Request form for the generic information that will apply to all subdivisions; and use separate forms for each new decimal subdivision, including on each form the information that is unique to that subdivision. If the course offered is less than a quarter or a term, please complete the Flexibly Scheduled/Off Campus/Workshop Request form.

Description (*not to exceed 25 words*): An introduction to computational chemistry including a survey of modern computational techniques and applications

Quarter offered: Fall Distribution of class time/contact hours: 3-1hr cl.
Quarter and contact/class time hours information should be omitted from Book 3 publication (yes or no):

Prerequisite(s): Chemistry 252

Exclusion or limiting clause:

Repeatable to a maximum of _____ credit hours.

Cross-listed with:

Grade Option (Please check): Letter X S/U ☐ Progress ☐ What course is last in the series? _____

Honors Statement: Yes ☐ No X GEC: Yes ☐ No X Admission Condition
Off-Campus: Yes ☐ No X EM: Yes ☐ No X Course: Yes ☐ No X
Embedded Honors Statement: Yes ☐ No X
Service Learning Course*: Yes ☐ No X *To learn more about this option, please visit http://artsandsciences.osu.edu/currofc/

Other General Course Information:
(e.g. "Taught in English." "Credit does not count toward BSBA degree.")

B. General Information

Subject Code 400506 Subsidy Level (V, G, T, B, M, D, or P) B
If you have questions, please email Jed Dickhaut at dickhaut.1@osu.edu.

1. Provide the rationale for proposing this course:
There is no undergraduate course which introduces computational chemistry, and the common software available for use. The course will focus on problem solving in chemistry using these programs and applied to training in computational science.

2. Please list Majors/Minors affected by the creation of this new course. Attach revisions of all affected programs. This course is (check one): ☐ Required on major(s)/minor(s) ☐ A choice on major(s)/minors(s)
X An elective within major(s)/minor(s) ☐ A general elective:

3. Indicate the nature of the program adjustments, new funding, and/or withdrawals that make possible the implementation of this new course.
None

4. Is the approval of this request contingent upon the approval of other course requests or curricular requests?

Yes ☐ No X List:

5. If this course is part of a sequence, list the number of the other course(s) in the sequence:_____

6. Expected section size: 25 Proposed number of sections per year: 1

7. Do you want prerequisites enforced electronically (see OAA manual for what can be enforced)? Yes X No ☐

8. This course has been discussed with and has the concurrence of the following academic units needing this course or with academic units having directly related interests (*List units and attach letters and/or forms*):
Not Applicable ☐
Ralph Regula School of Computational Science run by the Ohio Super Computing Center

9. **Attach a course syllabus that includes a topical outline of the course, student learning outcomes and/or course objectives, off-campus field experience, methods of evaluation, and other items as stated in the OAA curriculum manual and e-mail to asccurrofc@osu.edu.**

Approval Process The signatures on the lines in ALL CAPS (e.g. ACADEMIC UNIT) are required.

1.	Academic Unit Undergraduate Studies Committee Chair	Printed Name	Date
2.	Academic Unit Graduate Studies Committee Chair	Printed Name	Date
3.	**ACADEMIC UNIT CHAIR/DIRECTOR**	**Printed Name**	**Date**

4. **After the Academic Unit Chair/Director signs the request, forward the form to the ASC Curriculum Office, 4132 Smith Lab, 174 West 18th Ave. or fax it to 688-5678. Attach the syllabus and any supporting documentation in an e-mail to asccurrofc@osu.edu. The ASC Curriculum Office will forward the request to the appropriate committee.**

5.	**COLLEGE CURRICULUM COMMITTEE**	**Printed Name**	**Date**
6.	**ARTS AND SCIENCES EXECUTIVE DEAN**	**Printed Name**	**Date**
7.	Graduate School (if appropriate)	Printed Name	Date
8.	University Honors Center (if appropriate)	Printed Name	Date
9.	Office of International Education (if appropriate)	Printed Name	Date
10.	**ACADEMIC AFFAIRS**	**Printed Name**	**Date**

Chemistry 644 Fall 2008

Lecture: TBA

Instructor: Richard Spinney
160B Celeste Lab 247-6847 spinney.2@osu.edu
Office hours: TBA

Textbook: Introduction to Computational Chemistry, 2nd Ed. Frank Jensen, Wiley

Additional reference materials in SEL include:
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 anf W.G. Richards
Encyclopedia of Computational Chemistry, Schleyer, P.v.R., Ed. (Vols 1-5)
Modeling Molecular Structures by Alan Hinchcliffe

A Guide to Molecular Mechanics and Quantum Chemical Calculations by Warren Hehre is available in the lab.

Prerequisites: Successful completion of Chemistry 252 (Organic Chemistry II)

Objectives: To provide a practical introduction to the theory and methods of molecular modeling and computational chemistry, focusing on its use for experimentalists. Hands-on experience will be obtained by all attendees in doing molecular mechanics, semi-empirical, *ab initio* quantum chemistry, density functional theory and modeling dynamic systems (molecular dynamics and kinetics).

Software: All students will be provided access to modern molecular modeling software (Gaussian03, Spartan, Chem3D and WebMO) in order to practice with computational chemistry. The software runs on PCs in the Computational Chemistry Instructional Facility (MP0008) and via the web (WebMO). Access to MP0008 will require a chemistry computer account and Buck ID for door access.

Grades: The final grade will be determined by your performance on weekly problem sets (50%), on two individual projects (10% each) and the midterm/final exam (30%).

The only exam for the course will be on the seventh week of the course.

Problem sets will be handed out in class on Wednesdays, and will be due the following Wednesday in class. For consistency, there will be no extensions on due dates.

For the problem sets, you must do all of the work yourself. You are welcome to discuss issues of how to do the calculations with other students, TAs or your instructor. However, you must do all of the calculations yourself, and submit the required written report. If there is any doubt, you will be asked to produce the output files for any calculation performed. (It would be advisable to keep all of your work until the end of the course.)

The course is meant to be a practical introduction to computational chemistry, so besides attending lectures and doing the problem sets, each student is expected to work on two small "research" style computational projects. The first project will be to rationalize the activities of one or more drugs based on their physical and chemical properties. This will be completed over the course of the first five weeks of class.

The second project is more open, hopefully based on a suggestion from the student. If you have difficulties coming up with a problem of interest, please discuss the matter with me, there are a number of continuing projects you may work on. You should start the second project by the fifth week of classes to be sure of completing it on time. The final written report (~ 5 pages long) is due by the last day of classes.

Schedule of lectures:

Week 1	Molecular Mechanics, Energy minimization techniques,
Week 2	Potential energy surfaces and conformational searching
Week 3	Ab initio theory, Hartree-Fock theory
Week 4	Basis sets
Week 5	Semi-empirical methods
Week 6	DFT methods
Week 7	Advanced correlation methods. QSAR
Week 8	Modeling chemical reactions, solvation
Week 9	Modeling solid state and large systems
Week 10	Dynamic systems: molecular dynamics and kinetics

Academic Misconduct:
It is the responsibility of the Committee on Academic Misconduct to investigate or establish procedures for the investigation of all reported cases of student academic misconduct. The term "academic misconduct" includes all forms of student academic misconduct wherever committed; illustrated by, but not limited to, cases of plagiarism and dishonest practices in connection with examinations. Instructors shall report all instances of alleged academic misconduct to the committee (Faculty Rule 3335-5-487). For additional information, see the Code of Student Conduct (http://studentaffairs.osu.edu/info_for_students/csc.asp).

Disability Services:
Students with disabilities that have been certified by the Office for Disability Services will be appropriately accommodated, and should inform the instructor as soon as possible of their needs. The Office for Disability Services is located in 150 Pomerene Hall, 1760 Neil Avenue; telephone 292-3307, TDD 292-0901; http://www.ods.ohio-state.edu/.

Christopher M. Hadad 688-3141 hadad.1@osu.edu

Chemistry 944 Spring 2007

Lecture: Monday/Wednesday/Friday 10:30 - 11:18 am 2017 McPherson Lab

Instructor: Professor Christopher M. Hadad
1033 Evans Lab 688-3141 hadad.1@osu.edu
100C Celeste Lab 292-1204
Office Hours: Monday: 2:30 – 4:00 pm 100C Celeste
Wednesday: 9:00 – 10:15 am 100C Celeste
Otherwise, stop by anytime (and often).

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

TA: Jeremy Beck (jbeck@chemistry.ohio-state.edu, 1042 Evans lab, 688-3339)

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

Other reference materials on reserve at the science and engineering library include:

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. Time permitting, we will explore molecular dynamics, ligand docking into active sites, and other topics.

Software: All students will be provided access to molecular modelling software (Gaussian03 from Gaussian, Inc., Spartan from Wavefunction, Chem3D from CamSoft, HyperChem from Hypercube, TurboMole and MacroModel) in order to practice with computational chemistry. The software will run on the PCs, Macs, and workstations in the Chemistry department as well as the Ohio Supercomputer Center.

Visualization will occur on graphic workstations in the center as well as on the Macs and PCs in the center. Access to networked PCs or Macintoshes will be useful but not necessary. The software and UNIX workstations will be made available by the Chemistry department. As long as one has access to a chemistry E-mail account

(username@chemistry.ohio-state.edu), then you have access to the workstations and the software for this class. If you do not have a Chemistry E-mail account, please see me as soon as possible to arrange access to these resources.

We have some 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 **midterm/final exam (30%)**.

The ONLY exam for the course will occur on:

Exam	**Saturday, May 26**	**9:00 am - 12:00 noon**	**2017 MP**

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 8 problem sets for the entire course. For consistency, there will be no extensions on due dates.

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).

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 -- 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 4-5th week of the quarter to present an abstract of the topic of your project/paper. 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 (10 - 20 pages) on this project should be written in the style of a paper to the *Journal of the American Chemical Society* or similar ACS journal, complete with introduction, methods, results, tables, figures, conclusions and references. The due date will be presented later (but probably due during the week of finals).

Your scores will be listed on Carmen at:

https://carmen.osu.edu

Dates: The last day to drop this course without receiving a "W" on your record is Friday, April 13. The last day to drop this course without having to file a petition is Friday, May 11.

Ohio Supercomputer Center

1224 Kinnear Road - Columbus, Ohio 43212-1163 - phone (614) 292-9248 - fax (614) 292-7168 - www.osc.edu

The Ralph Regula School of Computational Science is an initiative of the Ohio Supercomputer Center

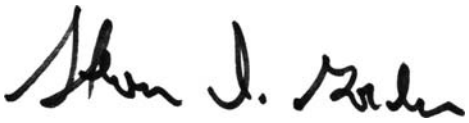
October 15, 2007

Dr. Christopher Hadad
Professor, Chemistry
The Ohio State University
88 W Eighteenth Avenue
Columbus, OH 43210
CAMPUS

Dear Chris,

I am writing to indicate my support for the creation of your undergraduate computational chemistry course, Chemistry 644. This course will fulfill the needs of the newly created statewide computational science minor program for the Ralph Regula School of Computational Science. The program currently involves nine institutions statewide and is likely to add three or four more institutions in the coming year. The computational chemistry offering will help us to recruit students from the participating community colleges as well as cross registrations from other four-year institutions. The course will also be a national model for the integration of computation into the STEM fields as a part of our on-going programs with the National Science Foundation and other national organizations.

Sincerely yours,



Steven I. Gordon, Senior Director
Education and Client Services
Director, Ralph Regula School of Computational Science
EM: sgordon@osc.edu
www.osc.edu