Submit original with signatures + 1 copy + electronic copy to UAF Governance. See http://www.uaf.edu/ugov/faculty/cd for a complete description of the rules governing curriculum & course changes.

TRIAL COURSE OR NEW COURSE PROPOSAL

<table>
<thead>
<tr>
<th>SUBMITTED BY:</th>
<th>Department</th>
<th>Chemistry &amp; Biochemistry</th>
<th>College/School</th>
<th>CNSM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prepared by</td>
<td>John Keller</td>
<td>Phone</td>
<td>474-6042</td>
<td></td>
</tr>
<tr>
<td>Email Contact</td>
<td><a href="mailto:fjkw@uaf.edu">fjkw@uaf.edu</a></td>
<td>Faculty Contact</td>
<td>(same)</td>
<td></td>
</tr>
</tbody>
</table>

1. ACTION DESIRED (CHECK ONE):
   - Trial Course
   - New Course [X]

2. COURSE IDENTIFICATION:
   - Dept: Chem & Biochem
   - Course #: 623
   - No. of Credits: 3

Justify upper/lower division status & number of credits:
The course requires advanced courses typical of B.S. in chemistry as prerequisite. Student’s final project should apply to his or her graduate thesis research. Use of literature for reading and reference. As the course number suggests, this is a course to equip first-year graduate students with advanced tools for research. It does not include or require advanced mathematical or quantum methods.

3. PROPOSED COURSE TITLE:
   - Molecular Modeling

4. CROSS LISTED?
   - YES/NO
   - No

(Requires approval of both departments and deans involved. Add lines at end of form for such signatures.)

5. STACKED?
   - YES/NO
   - No

6. FREQUENCY OF OFFERING:
   - Alternate Spring
   - (Every or Alternate) Fall, Spring, Summer – or As Demand Warrants

7. SEMESTER & YEAR OF FIRST OFFERING (if approved):
   - Spring 2010

8. COURSE FORMAT:
   - NOTE: Course hours may not be compressed into fewer than three days per credit. Any course compressed into fewer than six weeks must be approved by the college or school’s curriculum council. Furthermore, any core course compressed to less than six weeks must be approved by the core review committee.

   - COURSE FORMAT: (check one)
     - 1
     - 2
     - 3
     - 4
     - 5 [X] 6 weeks to full semester
   - OTHER FORMAT (specify)
   - Mode of delivery (specify lecture, field trips, labs, etc)
   - Lecture and laboratory practicum

9. CONTACT HOURS PER WEEK:
   - 2 LECTURE hours/week
   - 0 LAB hours/week
   - 3 PRACTICUM hours/week

   Note: # of credits are based on contact hours. 800 minutes of lecture=1 credit. 2400 minutes of lab in a science course=1 credit. 1600 minutes in non-science lab=1 credit. 2400-4800 minutes of practicum=1 credit. 2400-8000 minutes of internship=1 credit. This must match with the syllabus. See http://www.uaf.edu/ugov/faculty/cd/credits.html for more information on number of credits.

[OTHER HOURS (specify type)]

Received
FEB - 4 2009
Dean's Office
College of Natural Science & Mathematics
10. **COMPLETE CATALOG DESCRIPTION including dept., number, title and credits (50 words or less, if possible):**

Chem 623 Molecular Modeling  Credits: 3 (2 + 0 + 3)

Theory and practice of quantum and molecular mechanics methods in organic, physical, inorganic, and environmental chemistry and biochemistry; applications of computational software on workstations and multi-processor servers.

11. **COURSE CLASSIFICATIONS:** (undergraduate courses only. Use approved criteria found on Page 10 & 17 of the manual. If justification is needed, attach on separate sheet.)

   - H = Humanities
   - N = Natural Science  [X]
   - S = Social Sciences

   Will this course be used to fulfill a requirement for the baccalaureate core?  [YES]  [X]  [NO]

   IF YES, check which core requirements it could be used to fulfill:
   - O = Oral Intensive, Format 6
   - W = Writing Intensive, Format 7
   - Natural Science, Format 8

12. **COURSE REPEATABILITY:**

   Is this course repeatable for credit?  [YES]  [X]  [NO]

   Justification: Indicate why the course can be repeated
   (for example, the course follows a different theme each time).

   How many times may the course be repeated for credit?  --- TIMES

   If the course can be repeated with variable credit, what is the maximum number of credit hours that may be earned for this course?  --- CREDITS

13. **GRADING SYSTEM:**

   LETTER:  [X]  PASS/FAIL:  [ ]

14. **REQUIREMENTS ON ENROLLMENT (if any)**

15. **PREREQUISITES**

   Graduate standing in chemistry or biochemistry; or one year each of undergraduate organic, physical, and analytical chemistry, or equivalent; or permission of instructor.

   These will be required before the student is allowed to enroll in the course.

   **RECOMMENDED**

   Inorganic chemistry

   Classes, etc. that student is strongly encouraged to complete prior to this course.

16. **PROPOSED COURSE FEES**  $45

   Has a memo been submitted through your dean to the Provost & VCAS for fee approval?  Yes/No  [Y]

17. **PREVIOUS HISTORY**

   Has the course been offered as special topics or trial course previously?  Yes/No  [Y]

   If yes, give semester, year, course #, etc.:  Spring 2004  Chem 494 3 cr Molecular Modeling

18. **ESTIMATED IMPACT**

   WHAT IMPACT, IF ANY, WILL THIS HAVE ON BUDGET, FACILITIES/SPACE, FACULTY, ETC.

   1. Increase in use of department computer lab, however no new facilities will be required.
   2. Temporary increase in use of computational servers at ARSC and chemistry department. Chemistry is installing one small server now, and plans a larger installation in the future. ARSC usage by students has precedent in previous trial course offering, which worked fine.
   3. Faculty time will be available due to dropping another graduate course (621).
19. **LIBRARY COLLECTIONS**

Have you contacted the library collection development officer (ffklj@uaf.edu, 474-6695) with regard to the adequacy of library/media collections, equipment, and services available for the proposed course? If so, give date of contact and resolution. If not, explain why not.

| No | Yes | X |

20. **IMPACTS ON PROGRAMS/DEPTS**

What programs/departments will be affected by this proposed action?

Include information on the Programs/Departments contacted (e.g., email, memo)

Potentially this course will be offered via video or Internet connection to the UAA campus. UAA students and faculty already have installed versions of HyperChem software as a result of an NSF grant to a consortium of UAF-UAA-UAS-MATsu chemistry departments. Also, students and faculty at UAA already have internet connectivity to ARSC computational servers. They will soon have internet access to UAF's WebMO server hosted in the Chemistry Department.

21. **POSITIVE AND NEGATIVE IMPACTS**

Please specify positive and negative impacts on other courses, programs and departments resulting from the proposed action.

No negative impacts have been identified.

Positive impacts: There is a strong unmet need identified by UAF Chemistry and Biochemistry Faculty for a course in molecular modeling and computational chemistry. As a result of taking this course, graduate students will have the practical training to apply molecular modeling methods to their own thesis projects. Also, theoretical methods provide models as basis for more convincing research proposals. Finally, solid computational chemistry capability in terms of hardware, installed software, student and faculty expertise contribute to the overall competitiveness and recruiting attractiveness of the department.

**JUSTIFICATION FOR ACTION REQUESTED**

The purpose of the department and campus-wide curriculum committees is to scrutinize course change and new course applications to make sure that the quality of UAF education is not lowered as a result of the proposed change. Please address this in your response. This section needs to be self-explanatory. Use as much space as needed to fully justify the proposed course.

Each year, as computing hardware and software become faster and more efficient, computational chemistry and molecular modeling methods take on increasingly important roles in the creation of scientific knowledge. More and more it behooves students to become well acquainted with, and proficient in, the most common methods and concepts so they can interpret information in the literature, and apply the methods in their own work.

This is a course for students in all areas of chemistry. It starts with a quick re-introduction to the practice of molecular modeling, then continues to advanced hands-on use of HyperChem and Gaussian software. Most of the student's time will be spent doing HyperChem calculations or running Gaussian jobs on an ARSC supercomputer, or other computational server. We will apply molecular modeling to problems in organic, inorganic, physical, analytical, and biochemistry.
## APPROVALS:

<table>
<thead>
<tr>
<th>Signature, Chair, Program/Department of:</th>
<th>Chem &amp; Biochemistry</th>
<th>Date 2-4-09</th>
</tr>
</thead>
<tbody>
<tr>
<td>Signature, Chair, College/School Curriculum Council for:</td>
<td>CNSM</td>
<td>Date 2/17/09</td>
</tr>
<tr>
<td>Signature, Dean, College/School of:</td>
<td>CNSM</td>
<td>Date 2/11/09</td>
</tr>
</tbody>
</table>

Signature of Provost (if applicable)

Offerings above the level of approved programs must be approved in advance by the Provost.

### ALL SIGNATURES MUST BE OBTAINED PRIOR TO SUBMISSION TO THE GOVERNANCE OFFICE

<table>
<thead>
<tr>
<th>Signature, Chair, UAF Faculty Senate Curriculum Review Committee</th>
<th>Date</th>
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</thead>
</table>

### ADDITIONAL SIGNATURES: (If required)

<table>
<thead>
<tr>
<th>Signature, Chair, Program/Department of:</th>
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<tbody>
<tr>
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<td>Date</td>
</tr>
<tr>
<td>Signature, Dean, College/School of:</td>
<td>Date</td>
</tr>
</tbody>
</table>
Syllabus  Chemistry 623  3 Credits (2+0+3)  Molecular Modeling

Instructor:  John Keller
Office:  161 NSF  Office hours: MWF 1-2 PM or by appointment
Contact:  474-6042 ffjwk@uaf.edu
Lecture:  T 11:30-12:30; R 11:30-12:30  165 NSF
Computer Lab Practicum:  T 12:30-3:30  163/172 NSF

Required Texts:
Computational Chemistry David Young 2002 ($70 used). A handy reference for all things computational chemistry-wise. Light on theory; heavy on practical advice.
Exploring Chemistry with Electronic Structure Methods, 2nd Ed. Foresman and Frisch, Gaussian, Inc. ($35 student price). Detailed information on using Gaussian with example input and output.
Computational Chemistry; HyperChem Reference; Getting Started; Chemist’s Developer Kit. All by Hypercube and available free in pdf format online in UAF Digital Chemistry Lab.

Catalog description. Theory and practice of quantum and molecular mechanics methods in organic, physical, inorganic, and environmental chemistry and biochemistry; applications of computational software on workstations and multi-processor servers.

Learning outcomes: After successful completion of this course, students should be able to (1) design modest computational chemistry projects using appropriate model chemistry, (2) carry out calculations on available UAF hardware, (3) critically interpret modeling results in terms of established chemical principles and a reading of the relevant chemistry or biochemistry literature, (4) present results in written form, as well as graphically and with various 3D visualization tools.

Literature Reading. Articles from the literature are available online and via SciFinder Scholar.

Prerequisites: Graduate standing, or one year each of organic and physical chemistry. Some experience using HyperChem or related programs is desirable.

Overview. Each year, as hardware and software become faster and more efficient, computational chemistry and molecular modeling methods take on increasingly important roles in the creation of chemistry knowledge. More and more it behooves students to become well acquainted, and even proficient in, the most common methods and concepts so they can interpret information in the literature, and apply the methods in their own work.

This is a course for students in all areas of chemistry. It starts with a quick re-introduction to the practice of molecular modeling, then most of the effort is spent on advanced hands-on use of HyperChem and Gaussian. Most of the student’s time will be spent doing calculations on a PC using HyperChem or running Gaussian jobs on an ARSC supercomputer, or other server. We will apply molecular modeling to problems in organic, inorganic, environmental, physical, analytical chemistry and biochemistry.

Course organization. There will be two lectures per week, plus a 2-hour lab which will be held in the Chemistry Computer Lab. During the lab students will work on molecular modeling exercises with any needed advice from the instructor.

Grading. Course letter grades will be based on scores (out of 110 points) on several molecular modeling project reports completed during the semester (~10 points apiece), plus a larger-scale research project that is hopefully related to their thesis research. The research project will result in a journal-style manuscript, a 20-min in-class presentation, and a 3.5’ x 3.5’ poster for presentation at the chemistry department end-of-the-semester poster potluck supper held at 4 PM on the Thursday before finals week.
<table>
<thead>
<tr>
<th>Total points</th>
<th>Projects</th>
<th>Research</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>80 (8)</td>
<td>Oral</td>
</tr>
<tr>
<td>Graduate</td>
<td></td>
<td>Paper</td>
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<tr>
<td></td>
<td></td>
<td>Poster</td>
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</table>

**Projects.** Projects will consist of answering a question concerning molecular structure using one or more calculation techniques, writing a report, and submitting log and/or structure files upon which the report is based. Overly-tardy reports will be penalized. **Report** grades will be based on quality of writing, thoroughness and lack of error in the calculation results, clarity of results presentation in graphical and tabular form, neat and written in good English.

**Topics.**
Basic theory of methods (molecular mechanics, semi-empirical, ab initio, density functional theory) general aspects only.
- Geometry optimization; Vibrational analysis; Definition and use of surfaces
- Natural bond order theory and practice
- Display and interpretation of MOs and NBOs
- Relationship of calculated energies and frequencies to thermodynamic quantities
- Modeling reactive intermediates: carbocations, carbanions, radicals, carbenes, etc
- Transition state structure and reactivity; Solvation; Conformational analysis
- Charge distribution – Mulliken population analysis and others
- Working with biomolecules: biomolecule force fields and mixed MM/QM calculations
- Visualization of biomolecules using Rasmol, Chime, or recent variations thereof
- Solid-liquid and solid-gas interfaces; metal complexes; molecular dynamics
- How to program HyperChem using Excel macros and HyperChem scripts
- Creating and interpreting HyperChem log files; Gaussian input and output files
- Using FTP, Telnet clients to run Gaussian jobs ARSC supercomputer
- Using GaussView to interpret Gaussian log files
- Using WebMO; Using NBO and NBOview
- Using SciFinder Scholar to find literature articles about molecular modeling
- Online computational resources

**Example project: Vibrational Analysis**
The basic carbonyl vibration occurs around 1700 cm\(^{-1}\), but this changes depending on what is attached to the carbonyl carbon. Design a series of 10 carbonyl-containing molecules to test the effect of some structural or electronic variable on the vibration frequency of the carbonyl group. Optimize and analyze these compounds using HC or Gaussian, and an appropriate QM method (no Gaussian Opt/Freq run should take more than 60 min). Formulate a “paper and pencil hypothesis” before you do the calculations, then compare your results to the hypothesis. Compare your results to the literature, both in terms of published experimental and theoretical studies.

**Warning:** Computers are fickle and unreliable. Start your projects early. Be persistent in trying various solutions to your problem. Do not expect machines to be working when you are trying to finish a project at the last minute. Also, job queues on computational servers everywhere become overloaded near the end of each semester, so plan accordingly.

**What this course does not cover:**
1. quantum mechanics in mathematical depth. I hope to provide enough quantum mechanical discussion in order to understand and define different kinds of semi-empirical and ab initio methods. If the student thirsts for more knowledge along these lines, the detailed discussions in optional texts are an excellent source.
2. coding methods, except for writing simple scripts for driving HyperChem and Gaussian.
3. Unix commands, except as necessary to log on to ARSC machines and run Gaussian calculations.
4. Other software packages such as Sybyl, GAMESS, NWCHEM, etc
Ethical Considerations: As a UAF student, you are subject to the UA Honor Code, which says in part:

"Students will not collaborate on any quizzes, in-class exams, or take-home exams that will contribute to their grade in a course, unless permission is granted by the instructor of the course. Only those materials permitted by the instructor may be used to assist in quizzes and examinations. Students will not represent the work of others as their own. A student will attribute the source of information not original with himself or herself (direct quotes or paraphrases) in compositions, theses, and other reports. No work submitted for one course may be submitted for credit in another course without the explicit approval of both instructors. Violations of the Honor Code will result in a failing grade for the assignment and, ordinarily, for the course in which the violation occurred. Moreover, violation of the Honor Code may result in suspension or expulsion."

Disabilities: Students with physical or learning disabilities are required to identify themselves to Mary Matthews in the Disability Services office, located in the Center for Health and Counseling (474-7043). The student must provide documentation of the disability. Disability Services will then notify the instructor of special arrangements for taking tests, working homework assignments, and doing lab work.

Schedule of Class topics and assignments. Assignments related to each topic will be handed out that week, and be due within about 2 weeks.

<table>
<thead>
<tr>
<th>Week</th>
<th>Topic (Lecture and related project)</th>
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<tbody>
<tr>
<td>1</td>
<td>HyperChem, Gaussian, WebMO How-To</td>
</tr>
<tr>
<td>2</td>
<td>Basic Theory and Practice of Mol Mechanics Methods</td>
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<tr>
<td>3</td>
<td>Basic Theory and Practice of Ab Initio Methods</td>
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<tr>
<td>4</td>
<td>Density Functional Theory</td>
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<tr>
<td>5</td>
<td>Optimization; Vibrational Analysis</td>
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<tr>
<td>6</td>
<td>Analysis of Transition State and reaction mechanism</td>
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<tr>
<td>7</td>
<td>Spring break</td>
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<tr>
<td>8</td>
<td>Solvation Methods</td>
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<tr>
<td>9</td>
<td>Surface computational and visualization (MO, ESP)</td>
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<tr>
<td>10</td>
<td>Molecular visualization software</td>
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<tr>
<td>11</td>
<td>Biochemical systems and special software</td>
</tr>
<tr>
<td>12</td>
<td>Inorganic systems, including surfaces</td>
</tr>
<tr>
<td>13</td>
<td>Special topics</td>
</tr>
<tr>
<td>14</td>
<td>Student presentations</td>
</tr>
<tr>
<td>15</td>
<td>Student presentations</td>
</tr>
</tbody>
</table>