The Department/School of _______ Chemistry and Biochemistry _______ requests permission to offer the following SPECIAL TOPICS course during the _______ Spring _______ term, 20_05_.

<table>
<thead>
<tr>
<th>Rubric</th>
<th>Course #</th>
<th>Section</th>
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<tbody>
<tr>
<td>CHEM</td>
<td>580</td>
<td>n/a</td>
</tr>
</tbody>
</table>

Title of Course

_Computational Chemistry: Molecular Modeling & Electronic Structure_

<table>
<thead>
<tr>
<th>Instructor</th>
<th>SSN</th>
<th>Capacity</th>
<th>Beginning Date - End Date*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dr. Robert K Szilagyi, assistant professor</td>
<td>406 994 4263</td>
<td></td>
<td>January 12 - April 29, 2005</td>
</tr>
</tbody>
</table>

Instructor’s email address: Szilagyi@Montana.EDU
Instructor’s phone number: 406 994 4263

<table>
<thead>
<tr>
<th>Credits**</th>
<th>Mode</th>
<th>Days</th>
<th>Times</th>
<th>Building</th>
<th>Room</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1 lect.+2 lab.</td>
<td>Mon + Wed</td>
<td>1-3 pm</td>
<td>Gaines</td>
<td>321</td>
</tr>
</tbody>
</table>

** If other than regular semester, indicate the dates and total contact hours
** Be specific regarding the number of credits. Do not list ranges (i.e. 1-5)

REQUIRED DOCUMENTATION FOR REVIEW OF 580 COURSES

A. Course Description:
1. What are the special goals or purposes of the course that support a “graduate” level of the course?
2. Is this course intended to be a required part of a new degree curriculum option, major, or minor?
3. Provide a course syllabus containing all major topics to be covered.
4. List required texts or other required references.

B. Level of Offering:
1. Has the course been offered previously as a 580?
   a. If so, when?
   b. What was the enrollment?
   c. What level of students took the course?
   d. What were the evaluations?
2. Does the course represent an upgraded version of an undergraduate level course?
   a. If so, how has the course been changed to justify offering it at the graduate level? (Be specific)
3. What are the prerequisites for this graduate course? (List exact MSU courses - e.g. ESCI XXX or equivalent)
4. What performance requirements are placed on students which make this a graduate course?
   a. Specifically state the written requirements or products of this course.
   b. How will the student=s learning be assessed and graded?

C. Relationship to other courses, curricula, and Departments:
1. Does this course build on or interrelate with other courses in your curriculum or related curricula?
   a. If so, which one(s)?
2. Does this course replace one or more courses that will not be offered?
   a. If so, which one(s)?
3. Do the topics in the proposed course duplicate or reiterate those in other courses in this or any other department?
   a. If so, how do the coverage and education experiences differ, and how are these duplications or reiterations justified?
4. When the course is to be co-sponsored, taught by faculty from more than one department, or when content overlaps areas of common concern, the concurrence of all department heads and deans involved must be indicated. What liaison has been conducted with other departments? State reactions, both favorable and unfavorable.

D. Students Served:
1. Does the proposed course serve:
   a. Majors only?
   b. Non-majors only? State area(s) or discipline(s) to be served.
   c. Both majors and non-majors? Indicate what specific efforts will be made to make the course materials relevant to all disciplines served. How are faculty and students in the other areas to be served being made aware of this course?
2. What is the anticipated course enrollment?

E. Resources (including instructor):
   1. Are department financial resources sufficient for offering this course?
   2. Does the instructor have the requisite academic training to offer this course?
      a. Describe these qualifications briefly and include a vita (if the instructor is non-tenured).
   3. Are the library holdings adequate to support this course?

F. Course Evaluation:
   1. How will the students evaluate the course and instructor?
   2. How will the department evaluate the course and instructor?

G. Previous Course Review:
   All courses must have received faculty review and approval by your college curriculum committee and dean before the College of
   Graduate Studies will consider them.

H. Other Supporting Material:
   Include any additional information you feel is needed to support this request.
A. Proposed Course (the Course) Descriptions:

1. The primary goal and purpose of the Course is to aid and promote critical thinking in terms of molecular principles in physical chemistry (in particularly thermodynamics, kinetics and spectroscopy), abstract quantum chemical definitions (electronic states, molecular orbitals, and electron spin) by allowing students to develop and graphically visualize the electronic wave functions and their various properties for molecular systems from their own research background. The planned molecular modeling exercises will help developing their stereoscopic visions and through colorful images and animations will bring physical chemistry closer to those students of preparative background. Potential energy surface studies on selected organic and inorganic reaction mechanisms will allow for demonstrating changes along a reaction coordinates in three dimensions and help with understanding various forms of chemical selectivity. The planned exercises are expected to improve the students' ability to generate chemical models as well as use them in quantitative analyses in their further research studies. Implementation of the Course into both undergraduate and graduate curricula will broaden the chemical knowledge and skills of current students, and hopefully increase chemistry enrollment by approaching students with computer science or biology interests in addition to chemistry.

2. The Course is not a required part of a new degree, curriculum option, major or minor. It is given to provide an additional opportunity for students to improve their chemical modeling and analysis skills.

3. The Course will cover a broad spectrum of computational chemical methods from molecular mechanics to integrated QM/MM simulations. The Course will meet twice a week. On Mondays, a lecture will be given about the theoretical background of each computational methodology. On Wednesday, case studies will be carried out demonstrating the application of each method discussed in the lecture. The outline of the 15-week course is as follows:

   i. Molecular graphics and molecular mechanics: database search in Protein Data Bank and Cambridge Crystallographic Database, analysis of protein active sites, hydrogen bonded network, biomimetic models
   ii. Stationary and dynamical structural optimizations: potential energy surface definition, conformational changes, protein folding, molecular dynamical simulations with explicit solvent molecules
   iii. Development of molecular mechanical forcefields: generation of a training set, definition of initial parameters, parameter space mapping strategies, fitting by internal/Cartesian coordinates
   iv. Semi-empirical Hamiltonians: introduction of electronic wave function, MNDO/AM1/PM3 Hamiltonians, examples to demonstrate physical pictures to various integrals and parameters, minimal valence basis set
   v. Extension of semi-empirical methods to transition metals: introduction of d-orbitals, PM3(tm), MNDO(d) methods, effect of parameter adjustment on the electronic structure, parameterization
   vi. Ab initio methods: HF and post-SCF methods: definition of MO, LCAO, Coulomb, exchange interactions, Slater determinant, basis set, perturbation theory, population analysis
   vii. Multireference calculations: examples, mixing of ground and excited states, active space definition, optimization of orbital and CI mixing coefficients, light harvesting bacteriorhodopsin system
   viii. Density functional theory: the workhorse of computational chemistry, quest for the divine functional, Kohn-Sham equation, non-interacting electrons, exchange-correlation functionals, analysis of electron density
   ix. Spectroscopic calibration of density functionals: correlation of spectroscopy and calculations, ground state methods: EPR, ENDOR, ESEEM, Mössbauer; excited state methods: EAS/CD/MCD, PhES, XAS
   x. Environmental effects, including solvent effects: polarized continuum models, hydrogen bonding, calculation of redox potential and pKa values, ligand strain and protein entatic states
   xi. Chain, lattice, crystals - periodic systems: modeling of periodic systems using boundary conditions, classical organic polymers, statistical thermodynamics of polymers, 1D-3D periodic systems, band structure
   xii. Integrated QM/MM methods: how to take advantage of each method, ONIOM multilayer approach, covalent interactions highest level, electrostatic intermediate, steric low, S-test and electronic embedding
   xiii. All atom modeling of metalloenzymes: ONIOM treatment of about 100 aminoacid containing protein with mononuclear site and crystal waters, structure, redox potential, spectroscopy: rubredoxins and cupredoxins
   xiv. Independent case studies. Final exam: presentation of the case studies
4. Most course-materials will be developed as *the Course* progresses using online resources (Computational Chemistry List at OSC, Quantum Chemistry Program Exchange at UI), electronic journals and databases, software user guides, and worked-out case studies.

B. Level of Offering:

1. *The Course* has not been offered previously as a 580 class.
2. *The Course* does not represent an upgraded version of any other course.
3. *The Course's* prerequisites are CHEM515 and/or CHEM533 for graduate and CHEM323-CHEM326 for undergraduates students. Equivalent courses will also be considered.
4. Students will conduct individual research projects in a selected or assigned topic and analyzing relevant literature independently. Specific examples will be provided in the class to demonstrate a method and its implementation; however, students are expected to apply each discussed computational method to their chosen topics. Evaluation will consist of in-class activity (20%), lab reports (50%), composition and presentation of a final paper (30%). The selected project will preferably be related to each student's research interest.
   a. Lab reports are required to be prepared in HTML or RTF formats and will be collected and evaluated electronically on a dedicated website. The reports are required to contain a concise summary of the underlying theory of an applied method, technical documentation of the performed calculations and a section of results and discussion.
   b. The in-class activity will be evaluated by how well the students execute the demonstrative examples, and what progress they make in their independent research project, while in class. The lab reports will be graded based on whether those convincingly show that students acquired the knowledge and gained the skills to carry a particular computational chemical investigation. The final presentations will have written and oral parts. Both the format and contents will be evaluated.

C. Relationship to other Courses, Curricula, and Departments:

1. *The Course* partially builds on CHEM515: Structure and Bonding in Inorganic Chemistry and CHEM533: Physical Organic Chemistry graduate courses, which are taught in the Fall semester.
   a. *The Course* can be considered as a continuation of the above courses in the form of hands-on calculations of geometric and electronic structures, visualizations of molecular symmetries respect to structures and orbitals, demonstrations of various bonding theories, potential energy surface mapping of selected organic and inorganic chemical transformations.
2. *The Course* does not replace any other course.
3. The topics in *the Course* overlap with parts of CHEM325 and CHEM326 undergraduate, and CHEM564 graduate courses to only a limited extent.
   a. The focus of both undergraduate and graduate courses mentioned in C.3. is very different than that of *the Course*. The CHEM325 and 326 courses use computational chemistry as an alternative tool to "measure" chemical properties without providing a detailed theoretical background. The CHEM564 course is the opposite, where the theory is discussed in great details with limited applications for small molecules. *The Course* aims for the middle by providing a theoretical background at sufficient level for recognizing the advantages and limitations of a given computational method and applying these on real size molecules from current chemical problems.
4. *The Course* is sponsored and taught by Dr. Robert K. Szilagyi, assistant professor at the Chemistry and Biochemistry Department. No conflict of interest or areas of common concern are known.

D. Students Served:

1. *The Course* serves all science majors and non-majors, in particular emphasize on Chemistry, Biochemistry, Biology, Physics and Mathematics. Upon approval, *the Course* will be advertised at the relevant departments (Computational Biology, Chemical Engineering, Physics, and Computer Science in addition to Chemistry and Biochemistry) and a formal discussion will be organized amongst the interested students before the end of the current semester.
2. The anticipated enrollment of *the Course* is between 5 and 8 graduate students (upper limit for the 8 available workstations); however, two undergraduate students have already indicated their intention to attend.
E. Resources:
   1. The Department's financial resources are sufficient for offering this course. In addition, the Computer Fee Committee of MSU awarded a $28,000 grant to establish a dedicated, Molecular Modeling and Design laboratory for the Course and additional computational chemical teaching activities of other courses.

   2. The instructor has the requisite academic training and extensive experience to teach the Course. Computational chemistry is the instructor's primary research area and he is planning to bring "hot, off-the-press" chemical problems into the classroom from his or other faculty's research activities.

   3. The library holdings through access to electronic journals and databases are sufficient for the start. The course materials (including a good textbook and reference books) will be selected as the Course develops. The instructor's library contains some of the most popular computational chemistry books, which will be made available for the students.

F. Course Evaluation:
   1. The students will evaluate the Course and the instructor using the standard evaluation forms provided by the Information Technology Center.

   2. Since most of the attendees of the Course will be graduate students already working with other faculty, the Course and instructor will be under a continuous evaluation by the department. In addition, the instructor will organize a mini-conference at the end of the class, where the students will present and discuss their independent research studies to the department.

G. Previous Course Evaluation:
   The introduction of the Course is a result of an ongoing discussion at the Department of Chemistry and Biochemistry, which resulted earlier in the submission of a successful Computer Fee Proposal. The faculty of the Department collectively supports the Course. The Course fits into the Department's long term plans as the research and education at the Department focuses on molecular level understanding of complex chemical and biological processes. The computational lab and the Course will provide the technical basis and the forum for disseminating the expertise, respectively, in studying organic and inorganic reactivities and selectivity, bioinorganic and bioorganic structure and function relationships at the molecular level.

H. Other Supporting material:
   During his graduate studies, the Instructor was involved in designing and executing a 5-year graduate program in chemical informatics at the University of Veszprém, Hungary. He taught Molecular Modeling and Molecular Design courses. The graduate program has been accredited by the Hungarian Academy of Sciences and now being offered at the University of Veszprém (contact: Prof. Lajos Benze ben016@almos.vein.hu).

   A discussion has been started with chemistry instructors at Bozeman High School with the intention to organize fun molecular modeling classes for high school students with chemistry interests (contact: Amy Washtak awashtak@bozeman.k12.mt.us).

   The approval of the Course would provide a possibility for the Instructor to gain experience to teach computational chemistry to an audience with diverse chemical and mathematical skills. This experience will be useful in organizing intensive hands-on short courses in computational chemistry during summers for high school and college teachers from around Montana including Tribal Colleges.