CHEM 4560/5560: Molecular Modeling
Fall 2014 (MWF 10-11, PS 138)

Instructor Information:
Instructor: Jan Kubelka
Office: Physical Sciences Building (PS) 321
Phone: 766-2673
Email: jkubelka@uwyo.edu

Office hours:
TR 3:30-5:00 pm and by appointment

Texts:
These are available as e-books from the UW library and will be occasionally used for reading assignments, exercises etc. There is no need to buy hard copies.
We will approximately follow this book, but as it is getting old, with significant changes and additions, which will be provided in the form of lecture notes/handouts.

Additional supplementary texts:

Course Website:
http://www.uwyo.edu/kubelka-chem/teaching.htm. Lecture notes, assignments, solutions and all relevant material will be posted.

Computers:
Computational exercises are a major part of this class. The computational software (Gaussian, NAMD, Tinker) runs on Chemistry Department machines under Linux operating system and will be accessed through ssh/sftp programs available on PC’s in student computer labs. Basic knowledge of Linux/Unix will be required. Graphical interface programs Gabedit (http://gabedit.sourceforge.net) and VMD (http://www.ks.uiuc.edu/Research/vmd/), installed on PC’s in the student labs, will be used for generating input and analysis of the output. These programs are free and can also be downloaded and installed on student’s personal computers. Computers are available for the class periods and will be also required for the assigned homework projects. The students can use the computers in PS138, their own personal ones or those in student computer labs on campus.

Course Description:
Emphasizes training in computational, electronic and vibrational structure, calculations ranging from molecular mechanics to semi-empirical to *ab-initio* methods.

Prerequisites:
CHEM 4507

Disability Statement:
If you have a physical, learning, or psychological disability and require accommodations, please let the instructor know as soon as possible. You must register with, and provide documentation of your disability to University Disability Support Services (UDSS) in SEO, room 330 Knight Hall.
Objectives/Outcomes/Standards
To successfully complete the course, students will be expected to:

(1) Have good practical knowledge and understanding of the molecular modeling principles and methods
(2) Have sufficient command of UNIX/Linux operating system
(3) Demonstrate proficiency with quantum chemistry (Gaussian) and molecular mechanics software
(4) Demonstrate proficiency with front end builder/visualization software
(5) Demonstrate ability to use the software to solve and evaluate real word chemistry problems

Students enrolled at 5000 level will be further expected to:
(6) Research and present topics from primary literature
(7) Apply the computational chemistry tools to solve independent research projects

Course requirements/Assignments:
The course is designed primarily as practical hands-on exercises in molecular modeling/computational chemistry, i.e. more of a laboratory than a lecture, although it will also include background/theory components. The students will be expected to read and study assigned material prior to classes, where it will be exercised and problems practiced. The preparedness and performance of the students during class will constitute a significant part of the grade, it is therefore essential that the students come prepared!
There will be weekly quizzes each Friday (starting the second week of classes) and the final exam, which will also constitute a significant part of the final grade.
Final exam is scheduled for Wednesday Dec. 12. The final will be comprehensive, addressing both theory and practical issues with molecular modeling/computational chemistry in general and the specific software used throughout the class in particular.

Additional Course Requirements for 5000-level Credit
For 5000 level credit, the students will be also required to 1) research and present the current topics from the primary literature, and 2) solve additional “homework” computational problems that will emphasize independent work.

Attendance:
Since the grade for this course will be based on in-class participation and weekly quizzes (vide supra) Attendance is mandatory! University sponsored absences are cleared through the Office of Student Life.

Grading:
Grades will be based on your performance during in-class exercises, weekly quizzes and the final exam:
A (≥90%), B (80-89%), C (60-79%), D (50-59%). The relative weighting of each component is given below.

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<thead>
<tr>
<th>Component</th>
<th>Weighting</th>
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<tbody>
<tr>
<td>In-class participation</td>
<td>100</td>
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<tr>
<td>Weekly quizzes (10 out of 12, 10 pts ea.)</td>
<td>100</td>
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<tr>
<td>Worksheets (about 15)</td>
<td>100</td>
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<tr>
<td>Final exam</td>
<td>100</td>
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<tr>
<td>Homework projects (5000 level)</td>
<td>100</td>
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<tr>
<td>Totals:</td>
<td>400 (4000 level)</td>
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<td>500 (5000 level)</td>
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