

**Structure and Energetics II**  
**CHEM 3320-1**  
**WINTER, 2013**

Instructor: Dr. Scott D. Pegan  
Rm: SGM 251  
Phone: 303-871-2533  
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Lectures: 9-9:50 am, MWF, Olin 103  
Office Hours: 10:00-11:00, F SGM 251

**Grading:** Midterm Exams      200 points  
              Project Presentation 100 points  
              Final Exam            100 points  
              Class Participation 100 points

The assignment of a letter grade to a given numerical grade will depend on the overall class performance. However, if everybody does well, grades will not be curved down. **Also, note that points will be deducted from your final grade for disruptive behavior.**

**Projected Grade Ranges** (unless revised lower by the instructor during the course):

A $\geq 94\%$	B- $\geq 80\%$	D+ $\geq 67\%$
A- $\geq 90\%$	C+ $\geq 77\%$	D $\geq 64\%$
B+ $\geq 87\%$	C $\geq 74\%$	D- $\geq 60\%$
B $\geq 84\%$	C- $\geq 70\%$	F $< 60\%$

**Exams:** There are 2 X 1 h midterm exams during the quarter, plus a 1 h cumulative final exam.

**THERE WILL BE NO MAKEUP EXAMS.** The only exceptions to the no-makeup policy will be for members of a university team or group, e.g. athletic team or music group scheduled to be away from campus at the time of the exam, and members of the U.S. Armed Forces with conflicting obligations. You must inform your instructor of this prior to the exam and make arrangements at that time for a makeup exam.

**Presentations:** A Group style research project with accompanying presentation. Dates will be announced after the first exam.

**Class Participation:** The instructor will determine this score for the overall effort the student demonstrates in class during in-class exercises, pre-class reading and discussions.

**Disability Services Program**

1. If you have a disability/medical issue protected under the Americans with Disabilities Act (ADA) and Section 504 of the Rehabilitation Act and need to request accommodations, please make an appointment with the Disability Services Program (DSP); 303.871.2372/ 2278/ 7432; located on the 4th floor of Ruffatto Hall; 1999 E. Evans Ave. Information is also available on line at <http://www.du.edu/disability/dsp>. See the Handbook for Students with Disabilities.

2. Any student who feels s/he may need an accommodation based on the impact of a disability should contact me privately to discuss your specific needs. Please contact the Disability Services Program located on the 4th floor of Ruffatto Hall; 1999 E. Evans Ave., to coordinate reasonable accommodations for students with documented

disabilities/medical issues. 303.871. / 2278 / 7432/ 2455. Information is also available on line at <http://www.du.edu/disability/dsp>; see the Handbook for Students with Disabilities.

3. If you qualify for academic accommodations because of a disability or medical issue please submit a Faculty Letter to me from Disability Services Program (DSP) in a timely manner so that your needs may be addressed. Disability Services determines accommodations based on documented disabilities/medical issues. DSP is located on the 4th floor of Ruffatto Hall, 1999 E. Evans Ave.; 303.871. 2372/ 2278 / 7432. Information is also available on line at <http://www.du.edu/disability/dsp>; see the Handbook for Students with Disabilities.

**DATE TOPIC\***

**WEEK 1 *In silico* versus *real-life***

Jan 7 Class Intro, benefits, computational resources

9 Chemical Coordination Systems

11 *ab initio* and Semi-empirical techniques

**WEEK 2 Energy Minimization and Force Fields**

Jan 14 Basis Sets

16 Applications of *ab initio* and Semi-empirical techniques

18 Small Molecules vs. Macromolecules (Molecule Mechanics)

**WEEK 3 Conformation Analysis**

Jan 21 Martin Luther King Holiday

23 Surfaces and Molecular Graphics

25 Applications Practice

**WEEK 4 Protein Structure Prediction I**

Jan 28 Exam I

30 Sequence Alignments I

Feb 1 Sequence Alignments II

**WEEK 5 Protein Structure Prediction II**

Feb 4 SS Prediction

6 Comparative and Threading Models I

8 Comparative and Threading Models II

**WEEK 6 Molecular Dynamics**

Feb 11 Molecular Dynamics I

13 Molecular Dynamics II

15 Docking programs I

**WEEK 7 *in silico* docking**

Feb 18 Docking programs II

20 Chemical library diversity

22 Exam II

**WEEK 8 Combinatorial Libraries**

Feb 25 Cheminformatics and Lead Identification

27 Pharmaceutical related tools I

Mar 1 Pharmaceutical related tools II

**WEEK 9**

Mar 4 Presentation Preparation

6 Project Presentation

8 Project Presentation

## **WEEK 10**

Mar 11 Project Presentation

13 Project Presentation

Mar 17 **FINAL EXAM** (comprehensive), 8-9:50 am, Olin 103

\*Daily Topics may change depending the progress of the class.

\*\*Exam will likely focus on these topics; however, the exact chapters covered will depend on the progress of the class.