

**Structure and Energetics II**  
**CHEM 3320-1**  
**SPRING, 2019**

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**Lectures:** 9-9:50 am, MWF, Olin 103

**Office Hours:** Monday - Friday (10:00-11:00) or by appointment

<b>Grading:</b>	Midterm Exams	100 points
	Final Exam	100 points
	Project I	100 points
	Project II	100 points
	Project III	100 points

Two exams will be given during the quarter a midterm and a final exam. Exam problems will be similar to the discussed in class and will cover task required for successful completion of the three assigned projects. Certain aspects of the projects will be assigned and therefore will be similar for all students; however, there will be some latitude for the student to choose their topic.

Week	Topic
	<b>Modeling of Chemical and Biochemical Data</b>
1	Building Models/ Applying Models to Data Analysis
	<b>Computations involving Macromolecules</b>
2	ab initio and Semi-empirical Techniques
3	Conformational Analysis/Structure Prediction
4	Molecular Dynamics
5	Molecular Dynamics Continued
6	Molecular Dynamics Continued
	<b>Electronic Structure of Small Molecules</b>
7	From Molecular Mechanics to Quantum Mechanics
8	Quantum Mechanics Continued
9	Molecular Geometry, Single Point Energy, and Geometry Optimization
10	Application to Chemical Reactions and Spectral Predictions

Software that will be used – Mathematica, Spartan/Gaussian, and Nanoscale Molecular Dynamics (NAMD)

**Projected Grade Ranges:**

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

**ACADEMIC DISHONESTY** While I advocate collaborative learning and teamwork, I also firmly believe that each individual should maintain the highest ethical standards in all of life's endeavors. As such, I support and will strictly enforce the Honor Code of the University of Denver. I have included the links for the Honor Code Statement and Honor Code Procedures for Students below. For further information, please see the Office of Citizenship & Community Standards' website at <http://www.du.edu/honorcode/statement.htm> for the Honor Code Statement and at <http://www.du.edu/honorcode/studentprocedure.htm> for the Honor Code Procedures for Students.