

M W 5:30 – 6:45 p.m.
Room: NS 128
Lab: Chemistry #111
TA: Karina Kornobis

MOLECULAR MODELING
CHEMISTRY 450

Prof: P. M. Kozlowski
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TEXT: Computational Chemistry: Introduction to the Theory and Applications of
Molecular and Quantum Mechanics, Errol Lewars, Kluwer Academic Publishers

TENTATIVE SCHEDULE (January 7, 2008)

Mon. January 7	Introduction to Molecular Modeling/Course Description/Grading
Wed. January 9	Concept of the Potential Energy Surface
Mon. January 14	Intro to the Schrödinger Equation; Born-Oppenheimer Approx.
Wed. January 16	Computational Chemistry; Geometry Optimization
Mon. January 21	Martin Luther King Day: NO CLASS
Wed. January 23	Molecular Mechanics
Mon. January 28	Question & Answer Session
Wed. January 30	Introduction to Spartan (LAB)
Mon. February 4	First Computational Project (LAB)
Wed. February 6	EXAM I
Mon. February 11	Computational Chemistry: Overview & Ab Initio Calculations
Wed. February 13	Introduction to Protein Data Bank and PyMol (LAB)
Mon. February 18	Basic Principles Density Functional Theory (DFT)
Wed. February 20	Second Computational Project (LAB)
Mon. February 25	Current DFT methods: the Kohn-Sham approach
Wed. February 27	Metalloenzymes (guest lecture Prof. C. A. Grapperhaus)
Mon. March 3	Final Project Assignment, Description and Demonstration
Wed. March 5	Third computational project (Lab)
Mon. March 10	SPRING BREAK
Wed. March 12	SPRING BREAK
Mon. March 17	Modern applications; DFT and transition metals
Wed. March 19	DFT – Inorganic Reaction Mechanisms
Mon. March 24	Final Project – Question and Answer session (Lab)
Wed. March 26	Final Project (Lab)
Mon. March 31	EXAM II
Wed. April 2	Final Lecture (selected topic)
Mon. April 7	Student Reports (6 per day) (two session)
Wed. April 9	Student Reports (6 per day) (two session)
Mon. April 14	Student Reports (6 per day) (two session)
Wed. April 16	Student Reports (6 per day) (two session)
Mon. April 21	Student Reports (6 per day) (two session)

Grading

The final grade will be based on three components: two exams, three computational labs and the final project.

1. Each Exam is worth 20 points = **40 points**
2. Each Computational Project is worth 10 points = **30 points**
3. The Final Project is worth 30 points for a grand total of **100 points**.

Scale

- A 100-90
- B 89-80
- C 79-70
- D 69-60

Class participation is required. If more than three classes are missed without the instructor prior knowledge, this results in a failing grade. Only medical absences will be accepted for make-up.

Office Hours

Dr. Kozlowski Monday and Wednesday 4:30 – 5:30 or by appointment
Karina Kornobis Friday 3:00-4:00