

## Advanced Physical Chemistry (CHEM 660)

Prof: P. M. Kozlowski  
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Tu Th 5:30 – 6:45 p.m.

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### TENTATIVE SCHEDULE

Tues. Aug. 21	Introduction/Course Description/Grading
Thurs. Aug. 23	Introduction to the Schrödinger Equation
Tues. Aug. 28	The Born-Oppenheimer Approximation
Thurs. Aug. 30	The Electronic Problem
Tues. Sept. 04	Many Electron Wave Function and Operators
Thurs. Sept. 06	Orbitals, Slater Determinants and Basis Functions
Tues. Sept. 11	Operators and matrix Elements, Spin Adapted Configurations
Thurs. Sept. 13	Harmonic Oscillator / Molecular Vibration
Tues. Sept. 18	The Hartree-Fock Approximation
Thurs. Sept. 20	Restricted Closed/Shell Hartree-Fock: The Roothaan Eqns
Tues. Sept. 25	Unrestricted Open-Shell Hartree-Fock: The Pople-Nesbet Eqns
Thurs. Sept. 27	<b>EXAM I</b>
Tues. Oct. 02	Configuration Interaction
Thurs. Oct. 04	Truncated CI and the Size-Consistency Problem
Tues. Oct. 09	The Multiconfiguration Self-Consistent Field (MCSCF) Method
Thurs. Oct. 11	Pair and Coupled-Pair Theories
Tues. Oct. 16	The Couple Cluster Approximation
Thurs. Oct. 18	Many-Body Perturbation Theory
Tues. Oct. 23	Integral Evaluation, Energy Analytical Derivatives
Thurs. Oct. 25	Geometry Optimization
Tues. Oct. 30	Location of Transition State
Thurs. Nov. 01	<b>EXAM II</b>
Tues. Nov. 06	Hohenberg-Kohn Theorems
Thurs. Nov. 08	Density Functional Theory (DFT) Derivation and Formalism
Tues. Nov. 13	Local and Non-local DFT
Thurs. Nov. 15	Time-Dependent Density Functional Theory
Tues. Nov. 20	Thanksgiving holiday
Thurs. Nov. 22	Thanksgiving holiday
Tues. Nov. 27	Selected Topic: Transition Metals - Density functional Theory
Thurs. Nov. 29	Selected Topic: Density Functional Theory and Spectroscopy
Thurs. Dec. 04	<b>FINAL EXAM</b>

## **Grading**

1. Each Exam is worth 30 points = **60 points**
2. The Final Exam is worth 40 points for a grand total of **100 points**.

## **Scale**

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

## **Office Hours**

Dr. Kozlowski            Tuesday and Thursday 4:30 – 5:30 or by appointment

## **Text:**

- A. Szabo and N. S. Ostlund, MODERN QUANTUM CHEMISTRY: Introduction to Advanced Electronic Structure Theory.
- I. N. Levine, Quantum Chemistry, Fifth Edition, Prentice Hall
- E. Lewars, Computational Chemistry, Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Kluwer Academic Publishers