

**CHEM\*3860 QUANTUM CHEMISTRY FALL 2006**  
**COURSE OUTLINE**

**Instructor:** Professor John D. Goddard  
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**Extension.** 53102 **Office:** 340 MACN

**Strongly Recommended Text:**

**Quantum Chemistry and Spectroscopy.**  
**T. Engel. Benjamin Cummings (2006).**

**Other Useful Texts:**

**Quantum Chemistry.**  
**D. A. McQuarrie. University Science Books (1983).**  
**Quantum Chemistry. 5<sup>th</sup> ed.**  
**I. N. Levine. Prentice Hall ( 2000)**

**Calendar Description:**

**CHEM\*3860 Quantum Chemistry F(3-1) [0.50]: Elementary quantum mechanics for the understanding of the electronic structure of atoms and molecules.**

**Topics:**

- 1. Historical Introduction. Schrödinger Equation. Postulates of Quantum Mechanics.**
- 2. Free Particle. Particle in One, Two, and Three Dimensional Boxes. Particle in a Box and the Real World.**
- 3. Operators. Commuting and Non-Commuting Operators. Measurement.**
- 4. Quantum Mechanical Models for Vibration and Rotation of Molecules. Harmonic Oscillator. Rigid Rotator. Angular Momentum. Vibrational Spectroscopy. Rotational Spectroscopy.**
- 5. Hydrogen Atom. Hamiltonian. Solution. Hydrogen Orbitals.**
- 6. Helium Atom. Electron Spin. Indistinguishability Electrons. Variational Method. Hartree-Fock Self-Consistent- Field Method.**
- 7. Hydrogen Molecule Ion. Hydrogen Molecule. Simple Molecular Orbital Theory. Bonding in Diatomic and Polyatomic Molecules.**
- 8. Computational Chemistry. Potential Energy Surfaces. Hartree-Fock. Theoretical Model Chemistries. Beyond Hartree-Fock. Gaussian Basis Sets.**

**Class Schedule:**

<b>Tutorial: Monday</b>	<b>13:30 – 14:20</b>	<b>MACN 201</b>
<b>Lectures: Monday Wednesday Friday</b>	<b>10:30 – 11:20</b>	<b>AXEL 028</b>

**Evaluation:**

<b>Problem Assignments</b>	<b>20</b>
<b>Mid Term Exam</b>	<b>20</b>
<b>(Probably during lecture time on Friday Oct. 27.)</b>	
<b>Computational Chemistry</b>	
<b>Projects</b>	<b>20</b>
<b>Final Exam</b>	<b>40</b>
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<b>TOTAL</b>	<b>100</b>