

# Structure & Bonding

*One must 1<sup>st</sup> learn atomic/molecular orbital theories to begin your understanding of molecular structure/reactivity and their interaction with light.*

*CHEM-4611*

*Fall '07*

**Purpose:** This course investigates and applies wave-mechanical models of bound electrons to account for the electronic structure of atoms and how it is used to explain the similarities/differences in the behavior of various elements in the periodic table. This is followed by the building of numerous molecular systems by applying Molecular Orbital Theory with Group theory and interpreting/predicting their electronic properties and chemical reactivity.

**Learning Outcomes:** Each student will acquire a basic understanding of the quantum mechanical view of multi-electron atoms and use this as a basis to build molecular systems, via *Valence Bond Theory*, *Molecular Orbital Theory* and *Group Theory*. Also, the student will be able to generate qualitative orbital energy diagrams for various molecular systems in such a manner that allows one to predict the electronic behavior and chemical reactivity. Finally, the student will have the ability to use computational software to build chemical systems and interpret the output based on the understanding of quantum mechanics.

<b>Instructor:</b>	<b>Professor Spencer Slattery</b>
<b>Phone:</b>	<b>(678) 839-6550</b>
<b>Email:</b>	<b><a href="mailto:sslatt@westga.edu">sslatt@westga.edu</a> (You must use your MyUWG address)</b>
<b>Office Hours:</b>	<b>Mon &amp; Wed (9:45 – noon; 1:15 - 3:45 pm); Room (2136)</b>
<b>Class Meetings:</b>	<b>Tues. &amp; Thurs. (2:00 - 3:15 pm):</b>
<b>Location:</b>	<b>TLC Building (Room 2105)</b>
<b>Text:</b>	<b>Reading Material will be provided.</b>
<b>Note:</b>	<b>General Chemistry, Inorganic and Physical Chemistry texts will be helpful for understanding the topics in this course.</b>

**Evaluation:** Your *course grade* will be computed as shown below.

A (90 - 100%); B (80 – 89%); C (70 – 79%); D (60 – 69%)	Percent of Total
*Exam #1 (Atomic Structure & Periodic Trends)	22%
*Exam #2 (Valence Bond & Molecular Orbital Theory)	22%
*Exam #3 (Molecular Symmetry & Group Theory)	22%
*Exam #4 (Computational Chemistry)	22%
Homework Assignments	12%
<b>Total</b>	<b>100%</b>

## Examinations

There will be four examinations along with homework assignments. The date of each test will be announced approximately two weeks in advance. **Cheating will not be tolerated. Any infraction will be taken before the disciplinary committee and played out to the fullest extent.**

## ***Topics to be covered!***

### ***I. Atomic Structure***

- A. Particle (Bohr) & Wave Mechanical Model of Single Electron Systems*
- B. Wave Mechanical Approximation of Multi-electron Systems*
- C. Periodic Trends based on Wave Mechanical Model*
- D. Spectroscopic Term Symbols (ground vs excited state)-*

### ***II. Valence Bond Theory***

- A. Lewis Dot Structure (geometry, resonance, & formal charge)*
- B. Valence Shell Electron Pair Repulsion Theory*
- C. Electronegativity & Bond Polarity*

### ***III. Molecular Orbital Theory***

- A. Valence Bond Theory vs Molecular Orbital Theory*
- B. Molecular Orbital Theory applied to Homo-Diatomic Systems*
- C. Molecular Orbital Theory applied to Hetero-Diatomic Systems*
- D. Molecular Orbital Theory applied to Triatomic Systems*

### ***IV. Group Symmetry applied to Molecular Orbital Theory***

- A. Symmetry Elements, Operators, & Character Tables*
- B. Molecular Orbital Energy Diagrams for Triatomic Systems*
- C. M.O. Energy Diagrams beyond Triatomic Systems*
- D. Spectroscopy & Selection Rules (the peculiar behavior of matter!)*
- E. Huckel MO Theory (a simple mathematical approach)*

### ***V. Computational Modeling of Molecules***

- A. Symmetries, Coefficients, and Eigenvalues*
- B. Molecular Orbital Energy Diagrams (HOMO & LUMO)*
- C. Extended Systems (Band Theory)*