## Syllabus Chemistry 571, Section 001 Theoretical Physical Chemistry MWF, 10:00 pm –10:50 am, Currens 202 Fall 2014

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Office Hours: MWF 11am - 12 non, Th 1 - 2pm; other times by appointment or when available.

**Textbooks**:

**Lecture:** *Quantum Chemistry*, **John Lowe & Kirk Peterson**, 3<sup>rd</sup> Edition.

**Prerequisite:** Chem 375 or equivalent.

Goals of the Course: In Chem 571, it is desired to give the student a more in-depth understanding of the basis of chemistry – Quantum Mechanics. Concepts such as bonding, reactivity and spectroscopy all stem from quantum theory. Thus, various quantum mechanical models, Molecular Orbital theory and some computational techniques such as the Self Consistent Field Method and others will be discussed. Completing the reading assignments on a timely basis is preferable and more rewarding than last minute cramming. The lecture will cover the following chapters:

- 1. Classical Waves and the Time-Independent Schrodinger Wave Equation.
- 2. Quantum Mechanics of Some Simple Systems.
- 3. The One-Dimensional Harmonic Oscillator.
- 4. The Hydrogenlike Ion, Angular Momentum and the Rigid Rotor.
- 5. Many-Electron Atoms.
- 7. The Variation Method.
- 8. The Simple Huckel Method and Applications
- 11. The SCF-LCAO-MO Method and Extensions.

Attendance Policy: Although strict attendance is encouraged, illnesses do occur. Keeping this in mind, students will be allowed to make up missed exams, quizzes and homework provided that the absence is an excused documented absence and is reports on the OARS system. Documentation must be given to the instructor within one week after the student returns to class.

**Definition of Excused Absences:** Excused absences include: Illnesses, documented family medical emergencies, military commitments, WIU required athletic trips, and other absences excused by the course instructor.

<u>Hour Examinations</u>: Two examinations will be given during the course, a midterm and a final. These two exams will count as 60% of the final grade.

September 29, Monday - Chapters 1 – 4 December 15, Wedmnesday - Chapters 5, 7, 8 & 11

**Final Examination:** A final examination will be given on Monday, December 15<sup>th</sup>, 2014 from 10:00 am to 11:50 am.

<u>Homework:</u> Since critical thinking and problem solving are important components of chemistry; homework will be assigned regularly in order to help students grasp principles and concepts discussed in class. Regular practice will help your overall exam scores. Homework will contribute 15% to total points.

Classroom Presentation: Each student will be required on a presentation appropriate to the course. Topics may come from research journals, scientific publications such as nature magazine as well as other sources so long as the content deals with the applications of quantum mechanics or computational chemistry. Students should check with the instructor in order to determine the appropriateness of the topic. Presentations will contribute 25% to the final grade.

**Grading:** Letter grades for the course will be assigned based on the following point system out of a maximum of 800 points:

$$A \ge 640 > B \ge 520 > C \ge 400 > D \ge 320 > F$$

## **Additional Required Expenses:**

A scientific calculator (including graphing calculators) is required for the course.

**Outside work requirements for the course**: Students are expected to study, review and learn all material discussed in lecture, as well as read assigned chapters in the textbook, and to work assigned practice problems/questions/terms listed in class or on Western Online. Generally a minimum of 2 to 3 hours of outside study time is required for each hour of class time for this course.

Chemistry Resource Center: Currens 107. Free tutoring and/or help is provided by the department through the Chemistry Help Center. General hours are 8:00 am - 5:00 pm, however the schedule posted outside of CH 107 should be consulted for specific days and times.

**WIU Policies:** It is the policy of Western Illinois University to accommodate individuals with disabilities pursuant to federal law and the University's commitment to equal educational opportunities. It is the responsibility of the student to inform the instructor of any necessary accommodations at the beginning of the course. Any student with a disability requiring accommodations should contact the Office of Disability Support Services.

In accordance with University policy and the Americans with Disabilities Act (ADA), academic accommodations may be made for any student who notifies the instructor of the need for an accommodation. It is imperative that you take the initiative to bring such needs to the instructor's attention, as he/she is not legally permitted to inquire about such particular needs of students. Students who may require special assistance in emergency evacuations (i.e. fire, tornado, etc.) should contact the instructor as to the most appropriate procedures to follow in such an emergency. Contact Disability Support Services at 298-2512 for additional services.

**Emergency Preparedness:** The WIU Office of Risk Management and Emergency Preparedness provides resources on how to respond to emergency situations. Please view the video resources at **www.wiu.edu/rmep/** (Click "Resources" on the right side of the page). If the fire alarms sound and/or students are asked to evacuate the building all students should proceed immediately to the nearest exit and gather at the <u>southwest corner of the Higgins parking lot (near the fence)</u> until the "all clear" is given. The following action is prohibited under the Student Conduct Code: Disorderly Conduct: Any behavior which disrupts the regular or normal functions of the University community, including behavior which breaches the peace or violates the rights of others. Any student convicted of academic dishonesty, can receive a failing grade and may be subject to further academic penalties. Web address for Academic Integrity Policy (<a href="http://www.wiu.edu/policies/acintegrity.php">http://www.wiu.edu/policies/acintegrity.php</a>)

Web address for Student Rights and Responsibilities: http://www.wiu.edu/provost/students/

**CLASSROOM POLICIES:** Other than a scientific calculator or laptop (for taking notes except during exams), data storage devices such as cell phones, IPODs and MP3 players <u>are not allowed</u> to be used in the classroom at any time!

All hats, caps, and hoods that cover your ears are not allowed to be worn during a quiz or exam. The instructor reserves the right to assign seating for the students during exams and/or any other time deemed necessary.

Exam grades are based on the total number of correct answers including partial credit. All grades are final. No curve will be applied to exam grades, and no "retakes" will be allowed. No "extra point" assignments will be made or applied to grades. Students can view their individual quiz and exam scores on Western OnLine (WIU ECom ID and password are required for login).

No incomplete will be given to a student with a failing grade in the course. No incomplete will be given in this course unless the student experiences a documented emergency that takes him/her away from the university for at least two consecutive weeks and/or causes him/her to miss the final exam. The student must notify the instructor of this emergency before the final exam.