**SYLLABUS – CHEM 532: ADVANCED PChem II**

**DATE LAST MODIFIED:** 8/22/17  
**CREDITS:** 3  
**TIME AND LOCATION:** MWF 12:10 – 1PM

**INSTRUCTOR:** Aurora E. Clark (Fulmer 275)  
**OFFICE HOURS:** Mondays and Wednesdays 1-2PM in Fulmer 275 and by appt.

**TEXTBOOK:** Frank Pilar “Elementary Quantum Chemistry” 1st edition (copies provided by Prof. Clark)  
**SUPPLEMENTAL TEXT:** Atkins and Friedman “Molecular Quantum Mechanics”

**COURSE OVERVIEW:** Chem 532 focuses upon the foundational elements of quantum mechanics and its applications to atomic and molecular systems. Connections will be made where appropriate to group theory, spectroscopy, molecular structure and reactivity.

**COURSE SCHEDULE:**

<table>
<thead>
<tr>
<th>WEEK</th>
<th>DISCUSSION AND PROBLEM SOLVING TOPICS</th>
<th>NOTES</th>
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| 1 (8/21-8/25) | Ch 1 Pilar  
Math review  
Pilar Ch 2.1-2.3 | IN CLASS PROBLEM SOLVING  
HW1 Assigned  
DO math review independently |
| 2 (8/28-9/1) | Ch 1 Pilar, Ch 2.4 -2.12 | IN CLASS PROBLEM SOLVING  
HW1 Due  
In-class quiz #1  
HW2 Assigned |
| 3(9/4-9/8) | Pilar Ch3  
**No Class M 9/4 Labor Day** | IN CLASS PROBLEM SOLVING  
HW2 Due  
In-class Quiz #2  
HW3 Assigned |
| 4(9/11-9/15) | Pilar Ch 4 | IN CLASS PROBLEM SOLVING  
HW3 Due  
In-class Quiz #3  
HW4 Assigned |
| 5(9/18-9/22) | Pilar Ch5 and begin Ch6  
**No Class MWF** | IN CLASS PROBLEM SOLVING  
Makeup Class Tuesday (TBD)  
HW#4 due over email |
<table>
<thead>
<tr>
<th>Week</th>
<th>Assignments</th>
<th>HW Due</th>
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<tbody>
<tr>
<td>6(9/25-9/29)</td>
<td>Pilar Ch 6 finish – end Exam 1 material</td>
<td>HW5 assigned</td>
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<tr>
<td>7(10/2-10/6)</td>
<td>Pilar Ch 7</td>
<td>In class problem solving Makeup Class (TBD) Exam 1 due HW6 assigned</td>
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<tr>
<td>8(10/9-10/13)</td>
<td>Pilar Ch 8</td>
<td>In class problem solving Makeup Class (TBD) HW#6 due HW7 assigned in-class quiz #5</td>
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<td>9(10/17-10/21)</td>
<td>Pilar Ch 8, Ch 9 No Class MW</td>
<td>In class problem solving Makeup Class (TBD) HW7 due HW8 assigned in-class quiz #6</td>
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<td>10(10/23-10/27)</td>
<td>Pilar 9-10 No Class WF</td>
<td>In class problem solving HW8 due HW9 assigned</td>
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<tr>
<td>11(10/30-11/3)</td>
<td>Pilar 11 End Exam 2 Material</td>
<td>In class problem solving Makeup Class (TBD) HW9 due HW10 assigned in-class quiz #6</td>
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<td>12(11/6-11/10)</td>
<td>Pilar Ch 12</td>
<td>In class problem solving HW10 assigned in-class exam #2</td>
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<td>13(11/13-11/17)</td>
<td>Pilar Ch 12-13</td>
<td>In class problem solving Makeup Class (TBD) HW10 due HW11 assigned in-class quiz #7</td>
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<td>14(11/20-11/24)</td>
<td>Thanksgiving Holiday Read Ch 15</td>
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<td>15(11/27-12/1)</td>
<td>Pilar Ch 15-16</td>
<td>In class problem solving Makeup Class (TBD) HW11 due HW12 assigned in-class quiz #8</td>
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<td>16(12/4-12/8)</td>
<td>Pilar Ch 18</td>
<td>In class problem solving Makeup Class (TBD) HW12 due</td>
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ASSIGNMENTS: As noted above, weekly homework is assigned and due at the beginning of class unless otherwise noted. Weekly quizzes will be given as a means to accumulate participation points and are open book. Exams will be a mixture of in-class exams and take home assignments.

STUDENT LEARNING OUTCOMES: Minimum Expectations for Students after taking Chem532 (Quantum)

1) Set up the time-independent non-relativistic Schrödinger equation for 1-dimensional systems (particle in a box, harmonic oscillator, particle on a ring, etc.), know the general form of the solutions and how to apply boundary conditions to create specific solutions (including normalization). Understand the physical outcomes of these solutions (e.g. tunneling)
2) Reasonably approximate the Hamiltonian for any system
3) Appropriately use commutation relations and operator algebra to understand the Heisenberg Uncertainty Principle, orbital and spin angular momenta (this includes the use of raising and lowering operators)
4) Be able to derive the energy expression for 1D and 2D systems (e.g. from PIB to spherically symmetric potentials, and given a specific type of $V(x)$ like a Morse potential)
5) Recognize and appropriately use the solutions/wave functions that are solutions to different systems (e.g. spherical harmonics, Hermite polynomials) for the determination of different physical properties (selection rules, energy of eigenstates, etc.)
6) Be able to apply perturbation theory to determine the $k$'th order corrections to energy and wave functions
7) Understand and correctly apply other approximation methods, like the independent particle approximation and the variational method to single and many electron systems
8) Be able to construct wave functions that are satisfy the Pauli Principle for a given atomic, or molecular system, assign the ground electronic state, and derive or identify the different contributions to energy for a many electron system (i.e. Coulomb, exchange integrals)
9) Understand and apply the appropriate approximations for many-atom systems (i.e. BO approx.)
10) Be able to use LCAO-MO theory to create electron configurations of molecules, employing the Aufbau principle to assign electronic states (including symmetry)
11) Understand and appropriately couple angular momenta to assign term symbols of atoms and molecules, understand the role of spin orbit coupling
**Grading**

*Participation points assessed through quizzes:* 25%
*HW:* 35%
*Exams:* 45%