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:
RED ITEMS – MISSED CLASSES AND MAKEUP CLASSES
BLUE ITEMS – EXAMS, HW, OR QUIZZES

WEEK	DISCUSSION AND PROBLEM SOLVING TOPICS	NOTES
1 (8/21-8/25)	CH1 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

		HW5 ASSIGNED
6(9/25-9/29)	PILAR CH 6 FINISH – END EXAM 1 MATERIAL	IN CLASS PROBLEM SOLVING MAKEUP CLASS (TBD) IN-CLASS QUIZ #4 HW5 DUE EXAM 1 ASSIGNED
7(10/2-10/6)	PILAR CH 7	IN CLASS PROBLEM SOLVING MAKEUP CLASS (TBD) EXAM 1 DUE HW6 ASSIGNED
8(10/9-10/13)	PILAR CH 8	IN CLASS PROBLEM SOLVING MAKEUP CLASS (TBD) HW#6 DUE IN-CLASS QUIZ #5 HW7 ASSIGNED IN-CLASS QUIZ #6
9(10/17-10/21)	PILAR CH 8, CH9 NO CLASS MW	IN CLASS PROBLEM SOLVING MAKEUP CLASS (TBD) HW7 DUE HW8 ASSIGNED
10(10/23-10/27)	PILAR 9-10 NO CLASS WF	IN CLASS PROBLEM SOLVING HW8 DUE HW9 ASSIGNED
11(10/30-11/3)	PILAR 11 END EXAM 2 MATERIAL	IN CLASS PROBLEM SOLVING MAKEUP CLASS (TBD) HW9 DUE IN-CLASS QUIZ #6
12(11/6-11/10)	PILAR CH 12	IN CLASS PROBLEM SOLVING IN CLASS EXAM #2 HW10 ASSIGNED
13(11/13-11/17)	PILAR CH12-13	IN CLASS PROBLEM SOLVING MAKEUP CLASS (TBD) HW10 DUE IN-CLASS QUIZ #7 HW11 ASSIGNED
14(11/20-11/24)	THANKSGIVING HOLIDAY READ CH 15	
15(11/27-12/1)	PILAR CH 15-16	IN CLASS PROBLEM SOLVING MAKEUP CLASS (TBD) HW11 DUE HW12 ASSIGNED IN-CLASS QUIZ #8
16(12/4-12/8)	PILAR CH 18	IN CLASS PROBLEM SOLVING MAKEUP CLASS (TBD) HW12 DUE

		IN-CLASS QUIZ #9 TAKE HOME FINAL ASSIGNED 12/8 DUE 12/15

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 SCHRODINGER 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 HAMILTIONIAN 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%