CHEM 658-001 Syllabus

Fall 2017

Instructor: Kathleen Gilbert, PhD, PE Department of Chemistry and Env. Science NJIT, Newark, NJ 07102 Email: <gilbert@njit.edu> Email is the best way to reach me	**Lecture and laboratory:** Tuesdays, 2:30 pm – 5:25 pm, 9/6/17 to 12/12/17, in Tiernan 110T. **NO SESSION on 11/21/17!** *50% lecture and 50% computer laboratory until the chapters are done. Project meetings will be during or outside of class to check student progress.* **Final presentations**: T 12/12/17 and TBD during final exam period.
Office: 368 Tiernan Hall Office hours: By appointment arranged after class or by email.	**Software required:** Spartan Student Edition, available in many NJIT computer labs. This does not need to be purchased, but it can be purchased from through Wavefunction.
TEXTBOOK: Quantum Chemistry, 7th Edition, by Ira Levine. (homework info for 5th and 6th edition provided). **YOU MUST ALSO PURCHASE:** A bound composition notebook for lab and project results. PLEASE make sure you know what this means; it must be BOUND with STRING NOT GLUED.	

Chem 658 - Advanced Physical Chemistry (3 credits)

Prerequisite: one year of undergraduate physical chemistry. Principles and applications of quantum chemistry; the wave equation, its properties and mathematics; the Schrodinger equation and wave functions; the harmonic oscillator; variational and perturbational methods; atomic theory, structure, and properties; simple molecules, LCAO and valence bond theories; semi-empirical methods; time dependence, and introduction to electronic and vibration-rotation spectroscopy.

Course Grading			
Exam 1	20%	Lab and project notebook	8%
Exam 2	20%	Project presentation	32%
Exam 3	20%	TOTAL	100%

MOODLE: There is a course Moodle site that will include significant resources and updates of importance to this course, both for the lecture and laboratory portions. Please check it frequently, and also make sure to check or forward your NJIT email in order to receive important announcements.

Notes on Exams

- All exams will be open book and open notes. Printouts of answer keys are expressly forbidden to be used. Exams during the semester will be 90 minutes, followed by a laboratory period or lecture.
- Exams must be completed in No. 2 pencil, and all work must be shown with scratch paper handed in. A non-programmable calculator may be used; no laptops or other electronic devices are allowed during exams.

Please review the NJIT Academic Integrity Code; any indications of cheating or other violation of the policy will be treated seriously according to NJIT policy and procedures.

Notes on Laboratory, Laboratory Notebook, and Project

- The 3-hour class period will be approximately 50% lecture and 50% lab for most weeks. The laboratory section will feature the use of the SPARTAN quantum mechanics package (Windows version), which is only available in certain computer laboratories including our regular classroom.

- Laboratory work will be supervised at the beginning of the semester, and unsupervised once projects are started. Team project meetings will be arranged, at least one meeting per project per week. Project meeting schedules will be worked out during the first class. PhD students will work alone; MS students must work in teams of two unless there is an odd number of MS students in the class. This is subject to computer availability in the classroom. Most of the project work will be done outside of the classroom.

- As noted above, students must purchase a bound "marble" notebook and bring it to class every week to record the results of the computer lab experiments and the individual research project. Every project meeting will involve showing me the latest results in the notebook. I will sign the pages of the notebook after each lab and project meeting to confirm that progress is being made and the notebook is being used.

- The notebook is meant to be a useful journal in which results are recorded. Pages should not be torn out and errors should be crossed out not erased. Results should be recorded directly in the notebook and not on written on individual pieces of paper and transferred to the notebook. Students will **not** be graded on neatness of the notebook (as long as it is readable), but rather on whether it is being used as a research tool. Points will be taken off the project grade if the notebook is not acceptable and/or missing information.

- There are materials on reserve for this course at the library that may be helpful in completing the laboratories and project. They should be reserved under Chem 658.

Notes on Project Presentations

- Projects will be submitted in Powerpoint .ppt or .pptx format via Moodle by the due date and time, and presented using the Powerpoint slides. It is recommended that students use their own laptop computer and keep their file on their hard drive. Be prepared to ask at least two questions on other presentations, or you will lose points on your presentation.

- The presentation will be live and not recorded. Each group member must present part of the work, and questions will be asked of each group member. The presentation should highlight the important parts of the poster and what you have learned.

- There should be 16 or more slides in each presentation. The submitted presentation should have 5 or more slides of raw (unmodified) data calculated using Spartan. Students who work together should each submit identical complete presentations covering the work of both students, not different presentations. More details will be provided later in the semester.

- Project topics will be chosen early in the semester, with each team being able to pick from a set of topics based on a random draw. MS students should make sure to select a partner early in the semester or one will be assigned. Lab projects will be done individually in all cases, not in a team.

COURSE SCHEDULE – CHEM 658 FALL 2017 GILBERT

***** indicates proposed exam date.

WEEK 1:	Tue 9/5	Introduction and Theory:Ch. 1 (The Schrödinger Equation) Lab #11: Conformational Isomerism in n-Butane
WEEK 2:	Tue 9/12	Theory: Ch.1 (The Schrödinger Equation) Lab #44: Addition of Singlet Difluorocarbene to Ethylene
WEEK 3:	Tue 9/19	Problem Set: Chapter 1 Theory: Ch. 2 (The Particle In a Box) Lab # 6: Substituent and Solvation Effects on Tautomeric Equilibria
WEEK 4:	Tue 9/26	Problem Set: Chapter 2 Theory: Ch. 3 (Operators) Lab #30 Aqueous pKa's of Organic Acids
WEEK 5:	Tue 10/3*	**EXAM 1: Chapters 1 and 2** Lab #5: IR Spectrum of CO_2, Acetic Acid and Benzoic Acid
WEEK 6:	Tue 10/10	Problem Set: Chapter 3 Theory: Ch. 4 (The Harmonic Oscillator) Project Work
WEEK 7:	Tue 10/17	Problem Set: Chapter 4 Theory: Ch.5 (Angular Momentum) Project Work
WEEK 8:	Tue 10/24	Problem Set: Chapter 5 Theory: Ch. 6 (The Hydrogen Atom) Project Work
WEEK 9:	Tue 10/31*	**EXAM 2: Chapters 3, 4, and 5** Project Work

*********** MONDAY November 6, 2017 – last day to withdraw ***********

WEEK 10:	Tue 11/7	Problem Set: Chapter 6 Theory: Ch.7 (Theorems of Quantum Mechanics) Theory: How to do a Powerpoint presentation Project Work
WEEK 11:	Tue 11/14*	Problem Set: Chapter 7 **EXAM 3: Chapters 6 and 7** Project Work
WEEK 12:	Tue 11/28	Project Work
WEEK 13:	Tue 12/5	Project Work
PROJECT PRESENTATIONS	Tue 12/12	**Students will present project Powerpoints. Students are required to attend all of both presentation sessions.**
PROJECT PRESENTATIONS	TBD	

HOMEWORK PROBLEMS: Please complete problems by the week following the associated lecture, as they will be reviewed the following week. They will not be collected or graded. You will need to demonstrate at least two problems on the board during the semester, and answer questions from the instructor or other students while you are at the board.

PROBLEM SETS (Ira N. Levine, *Quantum Chemistry*)

Assignment	5^{th}Ed	6^{th}Ed	7^{th} Ed
Chapter 1	1.12, 1.22	1.13, 1.23	1.15, 1.25
Chapter 2	2.2, 2.5, 2.7,2.15	2.2, 2.6, 2.9,2.15	2.3, 2.7, 2.10, 2.17
Chapter 3	3.23 (a,b), 3.27 (a,b), 3.36, 3.39	3.25 (a,b), 3.31 (a,b), 3.42, 3.45	3.23 (a,b), 3.30 (a,b), 3.44, 3.48
Chapter 4	4.12, 4.16, 4.17, 4.18, 4.20, 4.22, 4.24, 4.27	4.10, 4.14, 4.15, 4.19, 4.16, 4.18, 4.23, 4.25	4.9, 4.13, 4.14, 4.15, 4.19, 4.20, 4.24, 4.26
Chapter 5	5.9, 5.14(b) 5.24, 5.25	5.10, 5.14 (b), 5.22, 5.28	5.10, 5.14 (b), 5.23, 5.30
Chapter 6	6.5, 6.17, 6.18, 6.30, 6.34	6.9, 6.21, 6.22, 6.34, 6.38	6.9, 6.23, 6.24, 6.36, 6.40
Chapter 7—Also do: 7.28 (3rd Ed.) Consider a particle in a nonstationary state in a one-dimensional box of length L with infinite walls. Suppose at time $t_0$its state function is the parabolic function $\Psi(t_0) = N \times (L-x)\ 0 \leq x \leq L$ where N is the normalization constant. If at time t_0 we were to make a measurement of the particle's energy, what would be the possible outcomes of the measurement and what would be the probability for each such outcome?	7.6, 7.9, 7.17,7.26	7.8, 7.9, 7.21, 7.30	7.8, 7.9, 7.22, 7.31

Attendance note: Although attendance is not explicitly required, students who miss classes will fall behind on their computer labs, which must be finished before students can start on their project.

PLEASE NOTE: THIS SYLLABUS IS SUBJECT TO CHANGE BASED ON MATERIALCOVERED, UNIVERSITY CLOSURES, AND OTHER FACTORS. EVERY ATTEMPT WILL BE MADE TO KEEP STUDENTS AWARE OF ANY CHANGES TO THE SYLLABUS.