Course: CH 333 Advanced Physical Chemistry
Semester: Spring, 2014

Professor: Carl Salter CHS 225 phone 625-7920

optional Text: P. W. Atkins & J. de Paula, *Physical Chemistry*, 8th Ed. W. H. Freeman Publishing Co., 2006
plus other handouts from POGIL materials on P Chem.

Course Objectives:
The Advanced Physical Chemistry course will cover modern theories and techniques in physical chemistry that are applied to many areas of chemical research. To this end, the two principle topics of the course will be computational chemistry and spectroscopy. All three modern techniques in computational chemistry, molecular mechanics, semi-empirical methods, and *ab initio* methods will be studied, and we will look at examples from the literature where these computational methods have been used in research applications. The wide variety of spectroscopic techniques used to analyze chemical systems will be examined, with particular focus on vibrational and rotational spectroscopy. Lasers and modern laser spectroscopy will also be covered.

Topics:

Molecular Symmetry Chapter 12 1,2,4,7,8,13,14

Computational Chemistry Handout

Rotational and Vibrational Spectroscopy Chapter 13 4,6,8,9,11,12

Electronic Spectroscopy Chapter 14 1,2,3,4,5,8,12

Lasers Handout, JMU laser workshop

Magnetic Resonance Chapter 15 1,2,3,4,5,6,7

Assignments and Evaluation:

Bio sketch of an early physical chemist 15%
Review *From Ostwald to Pauling : the Making of a Science in America,* author John W. Servos. Select a physical chemist from the book and write a brief biographical summary of his life and work. You should include at least two

other references besides the book. You must clear your choice with me; two students can not have the same chemist. Choose your chemist by Jan 24; paper due Feb 28.

Reports on Electronic Structure Calculations 20%
Through out the semester there will be required calculations that you will perform using Gaussian using WebMO. You must submit written summaries of your results.

Review of physical chemistry paper on graphene 15%
From the primary literature, review one paper on an aspect of the physical chemistry of graphene (or its derivatives). The publication date of the paper should be after January 2010. First draft by Feb 13, final draft April 25.

Exam Mid-term Exam 20%

Final Exam 30%

It is within the instructor's purview to apply qualitative judgment in determining grades for an assignment or for the course.

Students who wish to request accommodations in this class for a disability should contact Elaine Mara, Assistant Director of Learning Services for Disability Support, 1307 Main Street (extension 1510). Accommodations cannot be provided until authorization is received from the office of Learning Services.