

FAYETTEVILLE STATE UNIVERSITY
DEPARTMENT OF NATURAL SCIENCES
COLLEGE OF BASIC AND APPLIED SCIENCES

Syllabus

Ψ^+ \rightarrow CHEM 322 \leftarrow Ψ^-

QUANTUM MECHANICS AND SPECTROSCOPY SPRING 2006

Lecture schedule: Tuesdays and Thursdays 2:00-3:15 PM, LS 304E

Lecturer: Dr. Jairo Castillo-Chará

Office: LS 321

Telephone: (910) 672-2062

Office Hours: MF 12:50-2:50 PM, T 4:00-5:00, R 12-2:00 and 4:00-5:00 PM, and by appointment

e-mail: jcastill@uncfsu.edu

Website: <http://faculty.uncfsu.edu/jcastill/>

1 MOTIVATION

You may ask yourself why do you should study quantum mechanics? The answer is that our industrial and technological worlds have evolved at to the point that the new promising developments will be in the nano and atomic size scales. Therefore we should learn to use quantum mechanics in order to be able to describe, understand and control things in the atomic world. For the chemists working in synthesis of organic or inorganic compounds quantum mechanics provide the means to understand mechanisms and dynamics processes through which reactions occur, biologists working with DNA can track the processes¹ in a given atom or group of this huge molecule by attaching a fluorophore to the group or atom that they want to study, then the fluorescence of the attached group can provide details of the dynamics in one section of the molecule. In the area of electronics and material science is worth to mention that a considerable number of new opto-electronic devices, semiconductor transistors and lasers will operate based on the laws of quantum mechanics. As new

¹S. Weiss, Science **283**,1676 (1999)

technology is developed in these areas, the new devices will considerably shrink in size at to the point that it is predicted that for the year to 2030 the cell size of random access memory devices will be less than the size of an atom.² This implies that a radical change in the science curriculum need to place in order to prepare science students with a background in quantum mechanics that will allow them to compete in the job market and to be able to contribute in the new developments of the science and technology of the future. This course is just a first attempt to provide the science students with a considerable background in the fundamental principles of quantum mechanics and some of its applications.

2 COURSE DESCRIPTION

This course is an attempt to present the essential ideas of quantum mechanics hopefully in a way that would be interesting, comprehensible and enjoyable to the students with a background of one year of college calculus and physics. The lectures in this class will cover non-relativistic wave mechanics, molecular spectroscopy and computational chemistry.

3 TEXTBOOK

1. David W. Ball, *Physical Chemistry*, Thomson Learning Inc, 2003
2. Engel E. and Hehre W., *Quantum Chemistry and Spectroscopy*, Pearson Education, Inc. San Francisco 2006.

4 ADDITIONAL READING

1. Peter Atkins and Julio de Paula, *Physical Chemistry*, 8th Ed., W. H. Freeman and Company, 2002. In this book you will find a very condensed treatment of quantum mechanics in chapters 11-14 and of molecular spectroscopy in chapters 16-18
2. Pauling , L. and E. B. Wilson, *Introduction to Quantum Mechanics*, New York: McGraw-Hill,

²A. F. V. Levi, *Applied Quantum Mechanics*, Cambridge University Press, Cambridge 2003.

1935. Although it is an old book written by a two nobel prize winner, you can still learn a lot from this book, you will find surprisingly a complete treatment of the harmonic oscillator and hydrogen atom explained in a way relevant to chemistry.

5 COURSE COMPETENCES

The course will allow students to develop analytical and problem solving skills to understand chemical bonding and radiation matter interactions by the efficient use of the basic models of quantum mechanics. More specific:

1. The students will be introduced to the practical implementation of quantum chemistry in chemistry through the use of molecular spectroscopy.
2. The present new exciting applications of quantum mechanics such as: scanning tunneling microscopy, quantum dots, teleportation and quantum computing will be introduced whenever possible making use of the most basic concepts.
3. Introduction to the modern theoretical methods to solve efficiently the non-relativistic Schrodinger's equation (Hartree-Fock, MP2) will be presented.

6 GRADES

This course will be graded on a maximum of 100 points distributed as follows:

Section	Points
Three hour Exams	45 Points
Final Exam	25 Points
Homework	15 Points
Quizes	15 Points
Total	100 Points

Your course grade will be determined using the total number of points that you have accumulated during the semester.

Percentile Points	Letter Grade
92 - 100%	A
83 - 91%	B
73 - 82%	C
64 - 72%	D
63 or less %	F

7 COURSE OUTLINE

Chapter	Description
9	Pre-Quantum Mechanics
10	Introduction to Quantum Mechanics
2	The Schrodinger's Equation (Thomas Engel's Book)
3	The Quantum Mechanical Postulates (Thomas Engel's Book)
11	Quantum Mechanics: Model Systems and the Hydrogen Atom
12	Atoms and Molecules
14	Rotational and Vibrational Spectroscopy
15	Introduction to Electronic Spectroscopy and Structure
16	Introduction to Magnetic Spectroscopy
16	Computational Chemistry (Thomas Engel's Book)

8 COURSE REQUIREMENTS:

This course assumes that the students have taken one year college calculus and physics. An introduction course to differential equations and linear algebra will be useful, however provisions will be made during the course to satisfy this requirements.