

9:00 – 10:15 pm, TR, Clark 166

Office: Bandelier East 108

Telephone: 277 1716

Email: hguo@unm.edu

Web: www.unm.edu/~hguo

Syllabus

In this course, we will discuss the quantum mechanical nature of molecular structure and bonding. We will start with a brief review of quantum mechanical principles, such as the Schrödinger's equation, the uncertainty principle, the wave-matter duality, and the superposition principle. We will illustrate these elemental principles in a number of simple examples, namely, particle in a box, harmonic oscillator, and rotors. The two commonly used approximations, namely the perturbation theory and variational principle, will be discussed. This is followed by a brief review of atomic orbital theory. We will then discuss the molecular orbital theory. The emphasis will be placed on simple diatomic molecules, but extensions to polyatomic molecules will also be addressed. The final part of the lecture will focus on the *ab initio* and semiempirical methods as well as density functional theory (DFT) in calculating molecular electronic structure.

The aim of this course is two-fold. First, the lectures outlined above prepare the student with the necessary background in quantum theory of molecular structure and bonding. Second and perhaps more importantly, we will teach the class the practical skills to compute molecular properties using *ab initio* and DFT programs such as the Gaussian.

Homework will be assigned on weekly basis. There will be two midterm exams, covering the materials discussed in the course. The final exam is in the form of a report of a Gaussian calculation project near the end of the semester. Each student is assigned a small molecule and asked to compute its properties using Gaussian 98. The final grade of a student will be judged based on the homework (15%), the two midterm exams (30% each), and the performance in the final report (25%).

The lectures will be based on a number of books, which are listed below:

References

Quantum Mechanics:

M. A. Ratner and G. C. Schatz, Introduction to Quantum Mechanics in Chemistry, Prentice Hall, 2001.

I. Levine, Quantum Chemistry, Prentice Hall, 1991.

L. Pauling and E. B. Wilson, Introduction to Quantum Mechanics, Dover, 1935.

P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, Oxford, 1997

C. E. Dykstra, Quantum Chemistry and Molecular Spectroscopy, Prentice Hall, 1991

Ab initio methods

W. J. Hehre, L. Radom, P. v. R. Schleyer, J. A. Pople, Ab Initio Molecular Orbital Theory, Wiley, 1986