

## 212009 – BASIC QUANTUM CHEMISTRY

CREDITS: 04 (four) – 60 hours/class

### CONTENT:

Fundamentals of Quantum Matrix Mechanics and subspace and base concepts and Hermitian operators. Application of Secular Equation and groups theory to obtain diagram of molecular orbitals from several molecules and discussion of physicochemical properties from the electronic structure.

### SYLLABUS:

1. Subspace and base.
2. Matrix description vectors of quantum operators.
3. Secular equation.
4. Hartree-Fock method, integrals of 1 electron and 2 electrons.
5. Concept of electronic correlation.
6. Application of the secular equation, using group theory to obtain molecular orbitals for H<sub>2</sub>, ethene, butadiene, water, ammonia, acetone, benzene, coordination compounds.
7. Difference between irreducible representation for orbitals and for total wave function.
8. Fukui's theory for frontier orbitals.
9. Woodward-Hoffmann rules.
10. Theory of disturbance and applications.
11. Fermi's Gold Rule and Electron Spectroscopy.
12. Selection rules.
13. Jahn-Teller Principle.
14. Photochemistry.
15. Correlation of electronic correlation and post-Hartree-Fock methods.
16. Introduction to Density Functional Theory.

### BIBLIOGRAPHY:

1. LEVINE, Ira N. Quantum Chemistry. 4.ed. Prentice Hall, 1991.
2. A. Fazzio, K. Watari, Introdução à Teoria de Grupos com aplicações em moléculas e sólidos, UFSM, Brasil, 1998.
3. A. Szabo, N. S. Ostlund, Modern Quantum Chemistry Introduction to Advanced Electronic Structure Theory, Dover Publications, INC, New York, 1996.
4. C. Cohen-Tannoudji, B. Diu, F. Laloë, Quantum Mechanics, Willey & Sons, Carlifornia, 1977.
5. Specific articles on quantum chemistry applications.