Program: Chemistry (15025012071P6)

Course: QUANTUM CHEMISTRY

Code: PPGQU0065

Workload: 60 hours

Credits: 04

Syllabus:

Time-Independent Schrödinger Equation; Time-Dependent Schrödinger Equation; Quantum Mechanics Theorems; Angular Momentum; Hydrogen Atom; Exact Solution of Schrödinger Equation for Hydrogenoid Atoms; Approximate Solutions for Schrödinger; Multi-electron Atoms; Pauli Exclusion Principle; Antisymmetric Wave Function: Slater Determinants; Norn-Oppenheimer Separation; Diatomic Molecules; Polyatomic Molecules; Electronic Structure of Diatomic Molecules; Electronic Structure of polyatomic Molecules; Molecular orbitals; Valence Bond Theory; Hartree-Fock Model Applied to Polyatomic Molecules; Quantum Chemistry Calculations; Av-Initio Methods; Semi-Empirical Methods.

Bibliography:

SIMONS, J.; Nichols, J. Quantum Mechanics in Chemistry. Oxford University Press Inc., New York, 1997.

LEVINE, I. N. Quantum Chemistry. Prentice-Hall International Inc., 4th Ed., New Jersey, 1991.

PILAR, FRANK L. Elementary Quantum Chemistry. Dover Publications, New York, 2001.

SZABO, A; OSTLUND, N. S. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory. Dover Publications, New York, 1989.

JENSEN, F. Introduction to Computational Chemistry. John Wiley & Sons, New York, 2002.

CRAMER, C.J. Essentials of Computational Chemistry: Theories and Models. 2nd ed., John Wiley & Sons, New York, 2002.

Recent articles published in indexed journals.