22SC807 Frontiers in Computational Chemistry 3 0 1 4

Objectives:

1. Provide understanding of different aspects of computational chemistry.

2. Describe knowledge of various approximate techniques in quantum chemistry.

UNIT-1

Introduction and Numerical Methods: Introduction, Basic Programming Techniques, Interpolation and Curve Fitting, Roots of Equations, Matrix Methods, Differential Equations, Numerical Integration, Integral Transforms

UNIT-2

Variational Principle, Variational Method: Linear Variational Method and applications. Variational Method in Chemical Bonding, Molecular Orbital Treatment of Polyatomics. Perturbation Theory - Molecular Response to Electric Field, Degenerate Perturbation Theory. Excited States of He Atom, Slater Determinants, Energy Expectation Value with Slater Determinants, Self-Consistent Field Method.

UNIT-3

Canonical Hartree-Fock Equations, Hartree-Fock Energy, Hartree-Fock-Roothan Equations. The Density Matrix, Evaluation of Molecular Properties, Basis Sets, Electron Correlation and Post Hartree-Fock Methods, Time-Dependent Perturbation Theory, Slowly Switched Constant Perturbation, Oscillating Perturbation, and Einstein's Coefficients.

UNIT-4

Density functional methods, Softwares for quantum mechanical calculations, Different forms of inputs for Ab initio calculations, Computation of single point energies

UNIT-5

Geometry optimization: Electron densities and electrostatic potentials, Analysis of output for Gausian programmes, Molecular frequencies, modelling in solutions, Thermodynamic functions, NMR frequencies, QSAR, Transition states

Reference Books

1. Kauzmann, W., 2013. Quantum chemistry: an introduction. Elsevier.
2. Levine, I.N., Busch, D.H. and Shull, H., 2009. Quantum chemistry (Vol. 6). Upper Saddle River, NJ: Pearson Prentice Hall.
3. Labanowski, J.K. and Andzelm, J.W. eds., 2012. Density functional methods in chemistry. Springer Science & Business Media.

Preparatory Course Material

1.Prof. Sabyashachi Mishra, Approximate methods in Quantum Chemistry, IIT Kharagpur, NPTEL Course Material, https://nptel.ac.in/courses/104105128

2. Computational Chemistry, IIT Bombay Prof. B.L. Tembe, Dr. Sanjoy Bandyopadhyay, Prof. Shachi Gosavi, Prof. Shankar Prasad Bhattacharyya, Prof. Dilip Kumar Maity, NPTEL Course Material, https://nptel.ac.in/courses/104101002