UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

CH3EO2 - COMPUTATIONAL CHEMISTRY (ELECTIVE) (3credits, 54 h)

Unit 1: Introduction to Computational Chemistry (9 h)

Theory, computation & modeling – Definition of terms; Need of approximate methods in quantum mechanics; Computable Quantities – structure, potential energy surfaces and chemical properties; Cost & Efficiency – relative CPU time, software & hardware; Classification of computational methods.

Unit 2: Computer Simulation Methods- I (9 h)

Introduction – molecular dynamics and Monte Carlo methods, calculation of simple thermodynamic properties - energy, heat capacity, pressure and temperature, phase space, practical aspects of computer simulation, periodic boundary conditions, Monitoring the equilibration, analyzing the results of a simulation, error estimation.

Unit 3: Computer Simulation Methods- II (9 h)

Molecular dynamics (MD) method – molecular dynamics using simple models – MD with continuous potentials, finite difference methods, choosing the time step, setting up and running a MD simulation; Monte Carlo (MC) method - calculating properties by integration, Metropolis method, random number generators, MC simulation of rigid molecules.

UNIT 4: ab intio Methods in Computational Chemistry (9h)

Review of Hartree – Fock method for atoms, SCF treatment of polyatomic molecules; Closed shell systems - restricted HF calculations; Open shell systems – ROHF and UHF calculations; The Roothan – Hall equations, Koopmans theorem, HF limit & electron correlation, Introduction to electron correlation (post -HF) methods.

UNIT 5: Density Functional Methods (9 h)

Introduction to density matrices, N-reprentability & V-represetability problems, Hohenberg – Kohn theorems, Kohn-Sham orbitals; Exchange correlation functionals

– Thomas-Fermi-Dirac model, Local density approximation, generalised gradient approximation, hybrid functionals; Comparison between DFT and HF methods.

UNIT 6: Basis Set Approximation (9 h)

Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, even tempered & well tempered basis sets, contracted basis sets, Pople-style basis sets and their nomenclature, correlation consistent basis sets, basis set truncation error, effect of choice of method/ basis set (model chemistries) on cpu time.

References:

1. C. J. Cramer, *Essentials of computational Chemistry: Theories and models,* John Wiley & Sons 2002.
2. Frank Jensen, *Introduction to Computational Chemistry,* John Wiley & Sons LTD 1999.
3. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
4. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real-World Problems"*, Wiley -Interscience, 2001.
5. Errol G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2 nd edn.*, Springer 2011.
6. I.N. Levine, *Quantum Chemistry,* 6th Edition, Pearson Education Inc., 2009.
7. P.W. Atkins & R.S. Friedman, *Molecular quantum mechanics*, 4th Edition, Oxford University Press, 2005.
8. W. Koch, M.C. Holthausen, *"A Chemist's Guide to Density Functional Theory"*, Wiley-VCH Verlag 2000.