CHN – 704 (E) Advanced Quantum Chemistry

Advanced Quantum Chemistry **60 Hrs (2 Hrs/week)**

(**Pre-requisite**: Mathematics at least up to First Year B.Sc. level is necessary. At least one PC among 4 students should be available)

I Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock Theory — 12 Hrs

Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater-Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Roothan equation, Gaussian basis sets

II Configuration Interaction and MC-SCF — 12 Hrs

Introduction to CI; full and truncated CI theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods.

III Semi- Empirical Theories — 12 Hrs

A review of the Hückel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MOPAC and AMI with hands on experience on personal computers.

iV Density Functional Theory — 12 Hrs

Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulation, N- and V-representabilities; review of the performance of the existing local (e.g. Slater Xa and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory.

V Computer Experiments — 12 Hrs

Computer experiments using quantum chemistry - software packages such as GAUSSIAN/GAMESS/MOPAC and modeling software e.g. MM2/ AMBER/CHARM etc.

Books Suggested

1 Modern Quantum Chemistry, N.S. Ostlund and A. Szabo, McGraw Hill.
2 Methods of Molecular Quantum Mechanics, R. McWeeny and B.T. Sutcliffe, Academic Press.
3 Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford.
4 Exploring Chemistry with Electron Structure Methods, J. B. Foresman and E. Frish, Goussian Inc.
5 Semi-empirical MO Theory, J.Pople and D.L.Beveridge.