GROUP - (C) ELECTIVE PAPER
PAPER II. ADVANCED QUANTUM CHEMISTRY

M.M. - 75 | 60 Hrs. (2 Hrs./Week)

Units	Topics
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 of 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 Huckel, 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.