Advanced Quantum Chemistry (CY60105)
Autumn Semester 2013-2014

Course of Study

1. **Introduction to Quantum Chemistry**
   Postulates and Principles of Quantum Chemistry; Exactly Solvable Models (PIB, HO, RR, H-atom); He atom; H_2 molecule; Born-Oppenheimer Approximation.

2. **Approximate Methods**
   Variational approach; Perturbation Theory (Time Independent and Time Dependent PT); PT for Degenerate States.

3. **Many-Particle Systems**
   Electron Spin; Antisymmetry Principle; Angular Momentum of Many-electron Systems; Spin orbital interaction; LS and JJ coupling; Atomic and Molecular Spectroscopic Term Symbols.

4. **SCF Method**
   Orbital Approximation; Slater Determinant; Slater Type Orbitals; Pauli's Exclusion Principles; HF-SCF Theory; HF-Roothan Equation; Restricted and Unrestricted HF; SCF Treatment of Water.

5. **One Electron Properties**
   Density Matrix; Mulliken charges and spin densities; Bond Orders; Dipole and Quadrupole moments; Electric Fields at the Nuclei; Local and Canonical Molecular Orbitals.

6. **Basis Functions**
   Gaussian-type Functions; STO-G Functions; Minimal, Full-Valence, and Split-Valence Basis Functions; Diffused and Polarized Functions; Correlation Consistent Functions; Effective Core Potentials.

7. **Electron Correlation from Post SCF Methods**
   CI Method; MP2 and Coupled Cluster Methods; Static and Dynamic Correlation; CASSCF, SA-CASSCF, RASSCF Methods; C(/R)ASPT2 Method.

8. **Density Functional Theory**
   Hohenberg-Kohn Theorem; Kohn-Sham Method; LDA, GGA Methods; Time Dependent DFT.

9. **Semi-Empirical Methods**
   $\sigma - \pi$ separation; Hückel Method; Pariser-Parr-Pople Method; Extended Hückel Method; CNDO, INDO, NDDO, AM1, PM3 Methods.

10. **Relativistic Quantum Chemistry**
    Klein-Gordon Equation; Dirac Equation; Coulomb-Breit-Pauli Operator; Dirac-Hartree-Fock Method; Foldy-Wouthoysen Transformation and Douglas-Kroll-Hess Transformation; Relativistic Effective Core Potentials and Core Polarization Potential.

11. **Solvent Effects**
    Self Consistent Reaction Field Models; PCM and COSMO Models.

12. **Applications of Quantum Chemistry and Comparison of Methods**
    Quantum Chemistry Softwares (Gaussian, Molpro, and Turbomole); Applications of Quantum Chemistry in (a) Molecular Spectroscopy (b) Chemical Reactivity, and (c) Enzyme Catalysis.