Quantum Chemistry and Dynamics

Graduate course CHEM-GA 2666
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This course is intended to provide a balanced presentation of both fundamental quantum dynamics theories as well as applications to realistic chemical dynamics problems primarily in gas-phase. It is intended for graduate students who already have grasped the fundamental theories of quantum mechanics. It describes the basic quantum theory and treatment for molecular systems for both electronic and nuclear degrees of freedom. The contents of the course are specially organized to contain two main parts: (1) Electron structure theory and (2) quantum theory for nuclear dynamics. The first part describes the fundamental theory of electrons including the basic Hartree-Fock theory and its underlying physical picture. This is followed by introduction of correlation methods including density functional theory and many-body perturbation theory, etc. The second part describes quantum mechanical treatment for nuclear dynamics. The time-dependent quantum treatment for molecular dynamics and theory of molecular interaction with radiation field are also described in the course.

Contents of the Courses:

1. Separation of Electronic and Nuclear Motions
2. Born-Oppenheimer Approximation
3. Hellmann-Feynman Theory
4. Diabatic Representation
5. Transformation between Representations
6. Crossing of Adiabatic Potentials
7. Hartree-Fock Theory
8. Restricted Hartree-Fock (RHF)
9. Unrestricted Hartree-Fock (UHF)
10. Koopman’s Theorem
11. SCF Solution of HF Equation
12. Electron Correlation
13. Multiconfiguration
14. Perturbation Methods
15. DFT
16. Vibrational motions of molecules
17. Discrete variable representation
18. Rotational motions of molecules
19. Spherical coordinates
20. Rovibrational motions of molecules
21. Time-dependent theory for nuclear dynamics
22. Interaction of molecules with radiation field
23. Time-dependent perturbation theory
Reference books:

1. Essentials of Computational chemistry Theories and Models, by Christopher Cramer.
2. Theory and Application of Quantum Molecular Dynamics, by John Zhang