Ph.D./M.Sc./B.Tech. Elective

CH 644 : Applied Quantum Chemistry (2-0-2-6)

Prerequisites : Basics Quantum Chemistry and Programming

Review of Quantum Chemistry: Molecular Schrödinger equation, Born-Oppenheimer approximation, variational principle, many-electron wavefunctions, Hartree-Fock theory and electron correlation, semi empirical theory; Some early density-functional theories: Thomas-Fermi model, Slater approximation of Hartree-Fock theory; Modern density-functional theory (DFT): Introduction to functionals and functional calculus, Hohenberg-Kohn theorems, Kohn-Sham approach, meaning and utility of the Kohn-Sham orbitals and eigenvalues, Approximate exchange-correlation functions; Practical DFT: Introduction to basis sets – localized and periodic basis sets, all-electron versus pseudopotential approximations, self-consistent methods to solve the Kohn-Sham equations. Hellmann-Feynman theorem and computation of forces, computation of electronic and structural properties; Introduction to a DFT code and some simple examples and case studies

Text Books

1. W. Koch and M. Holthausen, *A Chemist's Guide to Density-functional Theory*, 2nd Edition, Wiley-VCH, 2001.
2. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry*, Dover Publications, 1996.
3. R. M. Martin, *Electronic Structure: Basic Theory and Practical Methods*, Cambridge University Press, 2004.
4. R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules,* Oxford Science Publications, 1995.

References

1. F. Jensen, *Introduction to Computational Chemistry*, 3rd Edition, Wiley, 2017.
2. J. Leszczynski, A. Kaczmarek-Kedziera, T. Puzyn, M. G. Papadopoulos, H. Reis, M. K. Shukla (Eds.), *Handbook of Computational Chemistry*, 2nd Edition, Springer, 2017.