

Department of Chemical Sciences

Graduate Course on Quantum Chemistry

Course Content

1. Review of classical mechanics, Origins of quantum theory: Black-body radiation, photoelectric effect, Compton effect, Frank-Hertz experiment, Wave-particle duality, Line spectra of atoms.
2. Time-dependent and time-independent Schrödinger equations, Wavefunctions, Observables, Operators, Expectation values, properties of operators. The uncertainty principle.
3. Quantum mechanics of the free particle, barrier penetration, quantum mechanical tunnelling, potential well, the particle in a box, the harmonic oscillator.
4. Factorization techniques for solving second order differential eigenvalue equations. Complete solution of Schrödinger equation of hydrogen atom. Derivation of selection rules from commutation relations.
5. Angular momentum. Spherical harmonics.
6. Approximate methods: Variation theory, time-independent perturbation theory for non-degenerate and degenerate states. Time-dependent perturbation theory, transition probability, multiphoton transitions.
7. Many electron systems. The anti-symmetry principle, spin orbitals, Slater determinants. Construction of spin-correct wavefunctions. Addition of angular momenta and atomic term symbols. Hartree-Fock self-consistent field method for atoms.
8. Molecular structure. The Born-Oppenheimer approximation. Linear molecules. Non-crossing rules.
9. Semi-empirical molecular orbital methods. Hückel MO theory. Piser-Parr-Pople method, CNDO method.
10. *Ab initio* calculations: An introduction

Instructor: Ranjan Das

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Venue: Lecture room AG80

Days: Mondays, Wednesday, and Fridays

Time: 10:00 hr to 11:15 hr

The first lecture starts on August 12, 2015.

Suggested textbooks:

1. **Elementary Quantum Chemistry**
by **Frank L. Pilar**, 2nd ed., New York, McGraw-Hill,
1990, also by Dover Publications
2. **Elementary Quantum Chemistry**
by **Frank L. Pilar**, New York, McGraw-Hill
3. **Quantum Chemistry, 2nd edition**
by **A. B. Sannigrahi**, Books & Allied, 2010
4. Introduction to Quantum Mechanics
by Linus Pauling and W. B. Wilson, New York, McGraw-Hill, 1935
5. Quantum Mechanics
by John L. Powell and Bernd Crasemann, Reading, Addison-Wesley, 1961
6. Quantum Chemistry
by Henry Eyring, John Walter and George E. Kimball, New York, John Wiley, 1963
7. Molecular Quantum Mechanics
by P. W. Atkins and R. Freidman, Oxford Univ. Press,
Fourth edition, 2007
8. Introduction to Quantum Chemistry
by Jay Martin Anderson, New York, W.A. Benjamin, 1969
9. Principles of Quantum Chemistry
by D. V. George, New York, Pergamon press, 1972
10. Quantum Chemistry
by Ira N. Levine, 4th ed., New Delhi, Prentice-Hall of
India, 1991
11. Atomic and Molecular Orbital Theory
by Peter O'D. Offenhartz, New York, McGraw-Hill, 1970
12. Principles of quantum mechanics: as applied to chemistry
and chemical physics
by Donald D. Fitts, Cambridge University Press, 1999