



PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	Name
QF535	Introduction to Quantum Chemistry

Vector
OF:S-2 T:004 P:000 L:000 O:002 D:000 HS:006 SL:004 C:006 AV:N EX:S FM:75%

Pre requirement	F 328
-----------------	-------

Summary

Historic account on the description of light and matter. The old quantum mechanics. The quantization of radiation energy and mechanics. The postulates of quantum wave mechanics. Application to simple systems. Quantum chemistry: atomic structures and the molecular structure of simple systems. The teaching of quantum chemistry: supervised activities.

Program

- I. **Historical aspects of physics.** The description of light and the structure of matter before the old quantum physics. The evolution of the theory conducted by the experimental evolution. Some experiments that the theory was unable to account for.
- II. **Foundations of the old quantum mechanics.** Planck, Einstein: the new description of electromagnetic radiation. Bohr: the quantization of mechanical energy, stationary states, radiative transitions, a quantum model for the hydrogen atom. Weaknesses of the Bohr model and attempts to deal with them.
- III. **Foundations of modern quantum chemistry.** De Broglie: wave-particle duality of matter and the experiments that detected it. Heisenberg and matrix mechanics. The wave mechanics of Schroedinger. The existence of the electron spin, and its absence in Schroedinger's theory. Dirac: linearization of the wave equation and the prediction and discovery of anti-particles.
- IV. **The postulates of non-relativistic quantum-mechanics.** Application to uni- and bi-dimensional systems. The hydrogen atom according to Schroedinger. Multi-electronic atoms. The Pauli exclusion principle and its consequences. The first thirty years of quantum mechanics, an integrated view.
- V. **Quantum chemistry:** The practical limits of the theory and the methods to overcome them; the approximation of independent particles. Fock, fermions, and multi-electronic atoms. Electronic correlation, The H_2^+ molecule and the nature of the chemical bond. Diatomic and polyatomic molecules. The LCAO method. Quantum chemistry for high-school education. Lewis structures and historical context. Pauling, hybrid orbitals, the diagram of orbital occupation. The valence bond theory.
- VI. **Supervised activities:** Teaching quantum chemistry at the high-school.

Bibliography

1. D.A.McQuarrie and J.D.Simon, Physical Chemistry: A Molecular Approach, University Science Books; 1a. Edição (1997).
2. Sebera, D.K., Estrutura Eletrônica e Ligação Química, Ed. Polígono, 1a Edição(1968)
3. Giberti, A., Origens históricas da física moderna, Fundação Calouste Goulbekian, 1a Edição (1982)
4. Gamow, G., Thirty Years that Shook Physics: The Story of Quantum Theory, Dover, Reprint, (1985)
5. Hoffman, B., The Strange Story of the Quantum, Dover, Reprint, (1985),

Evaluation criteria

Critérios de avaliação definidos pelo Professor, com base no disposto na Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina, do Regimento Geral de Graduação. Frequência: 75 % (* O abono de faltas será considerado dentro do previsto no capítulo VI, seção X, artigo 72 do Regimento Geral de Graduação)