Code: **QF535**

Name: **Introdução à Química Quântica**

Name in English: **Introduction to Quantum Chemistry**

Name in Spanish: **Introducción a la Química Cuántica**

Subject type: **Weekly**

Approval Type: **Grade and Attendance**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semester / 2nd Period - even periods**

Requires Final Exam: **Yes**

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
4	**-**	**-**	**2**	**-**	**-**	**4**	**15**	**6**

Occurrence on curriculum: **05, 56**

Pre requirement: **F 328**

Summary: **Historical evolution of the description of light and matter. The old quantum mechanics, quantization of radiation energy, and mechanics. The postulates of wave quantum mechanics. Applications to simple systems. Quantum chemistry: atomic structures and molecular structures of simple systems. Teaching quantum chemistry: guided activities.**

Programa:

I. Historical aspects of physics, description of light and matter structure before old quantum physics. The theory's evolution is driven by experimental evolution. Some experiments that theories could not model.

II. The foundations of old quantum mechanics, Planck, Einstein: the new description of electromagnetic radiation; Bohr: quantization of mechanical energy, stationary states, radiative transitions, a quantum model for the H atom; Failures, weaknesses, and attempts to correct Bohr's model.

III. The foundations of modern quantum chemistry, De Broglie: duality, matter waves and the experiments that detected them; Heisenberg and matrix mechanics; Schroedinger's wave mechanics; The existence of electron spin and its absence in Schroedinger's theory; Dirac: linearization of the wave equation, prediction and discovery of antiparticles;

IV. The postulates of non-relativistic quantum mechanics, Applications to simple one and two-dimensional systems; The H atom according to Schroedinger; Multi-electronic atoms; Pauli Exclusion Principle and its consequences; The first thirty years of quantum mechanics, an integrated view.

V. Quantum Chemistry - Practical limits of the theory and methods to circumvent them; Hartree and the independent particle approximation; Fock: fermions and multi-electronic atoms; Electronic correlation; The H2+ molecule and the nature of chemical bonding; Diatomic and polyatomic molecules: the LCAO method; Quantum chemistry taught in high school: Lewis structures and their historical context. Pauling, hybridization, and orbital occupancy diagram. Valence bond theory.

VI. Guided Activities: Teaching quantum chemistry in high school.

Basic Bibliography

1) MCQUARRIE, D. A.; SIMON, J. D.; **Physical Chemistry: A Molecular Approach**; University Science Books, New York (1997).

2) LEVINE, I. N.; **Physical Chemistry**; McGraw Hill, New York, 6a ed. (2008)
3) MARTINS, R. A.; ROSA, P. S.; **História da Teoria Quântica**; Editora Livraria da Física, São Paulo (2014).

Supplementary Bibliography

1) GIBERTI, A.; **Origens Históricas da Física Moderna**, Fundação Calouste Goulbekian, São Paulo (1982)
2) GAMOW, G.; **Thirty Years that Shook Physics: The Story of Quantum Theory**, Dover, New York (1985)
3) HOFFMAN, B.; **The Strange Story of the Quantum**, Dover, New York (1985),
4) FEYNMAN, R.; **A Estranha Teoria da Luz e da Matéria**, Editora Senai, São Paulo (2018).
5) PIZA, A. F. R. T; **Schrödinger & Heisenberg: A Física Além do Senso Comum**; Odysseus Ed., 2ª ed., São Paulo (2007).
6) VALADARES, E. C. **Newton, A Órbita da Terra em um Copo D'água**; Odysseus Ed., São Paulo (2007).
7) GAVROGLU, K.; SIMÕES, A.; **Neither Physics Nor Chemistry: A History of Quantum Chemistry**, MIT Press, New York (2011).