Code: **QF536**
Name: **Química Quântica**
Name in English: **Quantum Chemistry**
Name in Spanish: **Química Cuántica**
Subject type: **Semanal**
Approval Type: **Nota e Frequência**
Characteristic: **Regular**
Frequency: **75%**
Period Type / Offering period: **Semestral / Todos os períodos**
Requires Final Exam: **Sim**

Vectors

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

Occurrence on curriculum: **05**

Pre requirement: ***MA311**

Summary: **Postulates of Quantum Mechanics. Schrödinger Equation. Exact solutions and approximation methods. Hydrogen atom and multi-electronic atoms. Electronic structure methods for molecular systems.**

Programa:

Historical Aspects. Wave properties: Wavelength, wave number; period, frequency, propagation velocity, amplitude. Fundamental equations of the old quantum theory: Planck and De Broglie.

I. First Postulate of Quantum Mechanics: Wave Functions: Stationary and time-dependent generic wave function. Probability density and probability. Normalized and non-normalized wave functions. Well-behaved wave functions: continuous, unique, and finite.

II. Second Postulate of Quantum Mechanics: Operators. Linear momentum operator. Creating operators from classical concepts: potential energy, kinetic, and Hamiltonian operators. Addition and multiplication of operators. Linear operators. Eigenvalue equation. Hermitian operators and orthogonal functions.

III. Some Fundamental Theorems. Orthogonality. Set of Orthonormal Eigenfunctions (Kronecker Delta). Expansion in a basis. Commutation. Heisenberg's Uncertainty Principle. Commutation of two operators in an eigenfunction set. - Orthogonality. Commutators and uncertainty principle.

IV. Third postulate: Mean Value Theorem. Mean values and probability for discrete and continuous values. Eigenvalues and mean values.

V. Fourth Postulate: Schrödinger Equation. Time-dependent Schrödinger equation. Separation of variables. Time-independent Schrödinger equation. Solution of the differential equation depending only on time. Global time-dependent wave function.

VI. Analytical solution of the particle in the one-dimensional box (1D). Recognizing the potential. Constructing the Hamiltonian and the Schrödinger equation. Analytical solution of the differential equation: The use of boundary conditions. Energy levels, wave function: normalization and nodes. Mean value of the momentum operator. Mean value of the position operator: mean value and most probable value.

VII. Analytical solution of the particle in the two-dimensional box (2D). Constructing the Hamiltonian and the Schrödinger equation. Separation of Variables. Degeneracy. Calculation of the mean value for more than one coordinate.

VIII. Analytical solution of the particle on the ring. Circular motion in the xy plane, construction of the kinetic energy operator: moment of inertia and angular momentum. Polar coordinate system and transformation of cartesian coordinates (xy) and polar coordinates (r,). Solution of the Schrödinger Equation and boundary conditions: energy quantization, degeneracy, association of quantum numbers with angular momentum on the z-axis.

IX. Rigid Rotor. Rigid rotor with two masses, center of mass for two bodies, changes of the origin of the coordinate system, representation of rotation kinetic energy in three dimensions: reduced mass, moment of inertia, and angular momentum. Angular momentum and construction of the angular momentum operator in cartesian coordinates. Polar spherical coordinates and transformation of the angular momentum operator coordinates. Solution of the Schrödinger equation for the rigid rotor, separation of variables and energy quantization. Wave functions of the rigid rotor: Associated Legendre functions and spherical harmonics. Association of quantum numbers with angular momentum.
X. Harmonic Oscillator. Classical solution of the harmonic oscillator: fundamental frequency and force constant. Solution of the Schrödinger equation for the harmonic oscillator involving two masses: The Hermite differential equation and energy quantization.
XI. Variational Principle and Perturbation Theory.
XII. H Atom and Multi-electronic Atoms.
XIII. Hartree Model. Definition of spin-orbitals and wave function as Hartree product using spin-orbitals. Determination of the mean value of electronic energy of a multi-electronic atom employing Hartree product. Integration over spin coordinates and the mean value of energy in terms of orbital functions. A simplified deduction of the Hartree method: independent particle model, orthonormal spin-orbitals, Coulomb integrals, and Hartree equations. Interpretation of Hartree equations: mean-field and self-consistent model. Fermions and bosons distributions: symmetry and anti-symmetry of the wave function. Wave functions for the He atom in the ground and excited states.
XIV. Hartree-Fock Method. Anti-symmetric Wave Functions for many electrons. Slater Determinants. Pauli Exclusion Principle.
XV. Molecular Orbital Theory.

Basic Bibliography

1) MCQUARRIE, D. A.; SIMON, J. D.; “**Physical Chemistry: A Molecular Approach**”; University Science Books, New York, 1997, 1360 p.
3) SALA, O.; “**Fundamentos da Espectroscopia Raman e no Infravermelho**”; 2ª ed., Ed. Unesp, 2011, 280 p.
3) BRAGA, J. P.; “**Fundamentos de Química Quântica**”; Editora UFV; Viçosa, 2007, 272 p.

Supplementary Bibliography

1) LEVINE, I. N.; “**Quantum Chemistry**”; 5a ed., Pearson, New York, 1999, 739 p.
2) BARROW, G. N.; “**Introduction to Molecular Spectroscopy**”; New York, McGraw-Hill Education, 1962, 318 p.
3) CHANDRA, A. K.; “**Introductory Quantum Chemistry**”; Tata McGraw-Hill, New York, 1994, 390 p.
4) LEVINE, I. N.; “**Physical Chemistry**”; 6a ed., McGraw Hill, New York, 2008, 1008 p.
5) DEMTRÖDER, W.; “**Atoms, Molecules and Photons: An Introduction to Atomic-, Molecular- And Quantum Physics**”; 2a ed., Springer, New York, 2010, 589 p.