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Instituto de Química
Graduate Program in Chemistry (Grade 7/CAPES)
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COURSE SYLLABUS

1. Identification

Code and title: QUP 143 – Methods in Electronic Molecular Structure
Professor: Paolo Roberto Livotto
Level: Master and Doctorate
Credit hours: 3
Revised: October_2019

2. Summary

Postulates of Quantum Mechanics. Wave functions for many electron systems. Hartree-Fock method. Base sets. Complete Base Set Templates. Electronic correlation. Methods for incorporating electronic correlation: Interaction of Configurations, Moller-Plesset Perturbation Theory and Coupled Clusters Theory. Density Functional Theory. Semi-empirical Methods.

3. Objective

Provide a knowledge concerning the fundamentals, concepts, approaches and methodologies related to the quantum mechanical description of molecular systems in the approximation of monoelectronic wave functions, in multiconfiguration methodologies and in approaches based on electron density.

4. Contents

4.1. Postulates of Quantum Mechanics. Hermitian operators and their properties.
4.2. Molecular Schroedinger Equation. Born-Oppenheimer Separation. Principle of Pauli. Determinants of Slater.
4.3. Hartree-Fock method. Hartree-Fock equations: Open and closed layer systems. Interpretation of the solutions of the Hartree-Fock Equations. electronic correlation
4.4. Roothaan-Hall Equations. Base function sets. Extrapolative and Additive Complete Base Set Models
4.5. Post-Hartree-Fock Methodologies: Configuration Interaction Method, Moller-Plesset Disturbance Theory and Coupled Cluster Theory.
4.6. Density Functional Theory. Hohemberg-Kohn theorems. Kohn-Sham equations. Exchange-correlation functionals.
4.7. Semi-empirical methods. ZDO approximation and derivatives. Parameterization Strategies.

5. Assessment

List of exercises, presentation and discussion of scientific articles, theoretical tests and/or directed works. The student, who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:
A: grade equal to or above 9.0
B: grade equal to or above 7.5 and below 9.0
C: grade equal to or above 5.0 and below 7.5
D: grade below 5
FF: lack of frequency

6. Methodology

Lectures, exercises lists, seminars and examinations.

7. Bibliography

- Attila Szabo and Neil S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Eletronic Structure Theory, McGraw-Hill, 1989.
- Nelson H. Morgon and Kaline Coutinho, Métodos de Química Teórica e Modelagem Molecular, Livraria da Física, 2007.
- Frank Jensen, Introduction to Computational Chemistry, 2ª ed, Wiley, 2007.
- Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, Wiley, 2004.
- Donald A. McQuarrie and John D. Simon, Physical Chemistry, University Science, 1997.