Universidade Federal do Rio Grande do Sul
Instituto de Química
Graduate Program in Chemistry (Grade 7/CAPES)
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COURSE SYLLABUS

1. Identification

Code and title: QUP 153 – Advanced Computational Chemistry
Professor: Paulo Fernando Bruno Gonçalves
Level: Master and Doctorate
Credit hours: 3
Revised: October_2020

2. Summary

Approach to the main methods involving Quantum Chemistry

3. Objective

Improve the student's knowledge of computational chemistry practices, having as a basic requirement, prior knowledge of basic computational chemistry at undergraduate level, quantum chemistry, and preferably, Methods of Electronic Structure of Molecules

4. Contents

- Principles of Structure and Properties of Molecules
- Introduction to Semi-empirical Methods
- Principles of Conformational and Vibrational Analysis
- Ab Initio Methods
- Comparison between Methodologies
- DFT: Comparison between Functionals
- Comparison between Load Distribution
- DFT calculations considering Solvent Effect
- Spectroscopy
- Surface of Electrostatic Potential and Orbitals
- Case studies: Reaction Mechanisms, Complexes, Periodic Systems, Chemical Reactivity, Aromaticity and Excited States

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.

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7. Bibliography

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- C. Cramer, Essentials of computational chemistry. New York: John Wiley, 2004.
- F. Jensen, Introduction to computational chemistry. San Francisco: John Wiley, 1999.
- J. M. Thijssen, Computational Physics, Cambridge Univ. Press. 2003.