Universidade Federal do Rio Grande do Sul
Instituto de Química
Graduate Program in Chemistry (Grade 7/CAPES)
Av. Bento Gonçalves, 9500 – Bairro Agronomia
Porto Alegre, RS – Brazil - ZIP 91501970
☎+55 (51) 3308 6258 – Fax +55 (51) 3308 7198
http://www.iq.ufrgs/ppgq - e-mail: ppgq_iq@ufrgs.br

# COURSE SYLLABUS

## 1. Identification

Code and title: QUP 011 – Advanced Classical Theoretical Chemistry
Professor: Paulo Augusto Netz
Level: Master and Doctorate
Credit hours: 3
Revised: August_2019

## 2. Summary

Fundamentals of Classical and Statistical Mechanics. Statistical thermodynamics in different ensembles. Statistical Thermodynamics of Real Gases and Liquids. Molecular dynamics, computational implementation and applications of molecular dynamics, Markov processes, Monte Carlo method. Brownian dynamics, hybrid methods.

## 3. Objective

Provide the students the theoretical foundations involved in classical computational experiments, such as molecular dynamics, Monte Carlo and other methods.

## 4. Contents

- Classical Mechanics: Initial Conditions, Equations of Motion, Separation of Molecular Degrees of Freedom
- Statistical Mechanics: Ensembles, Partition Function, Distribution Functions
- Statistical thermodynamics in different ensembles, transformations between ensembles
- Intermolecular interactions. Statistical Thermodynamics of Real Gases and Liquids
- Deterministic Computational Simulation: foundations of Molecular Dynamics. MD in the NVE, NVT and NPT ensembles. Methodological details, implementation, computational applications, advanced methods.
- Fundamentals of the Monte-Carlo method. Markov chains, ergodicity, rules of acceptance. Computational implementation. MC in different ensembles. Applications
- Advanced method.

## 5. Assessment

Solution of exercises, exam and presentation of recent relevant articles from the literature. 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.

Universidade Federal do Rio Grande do Sul
Instituto de Química
Graduate Program in Chemistry (Grade 7/CAPES)
Av. Bento Gonçalves, 9500 – Bairro Agronomia
Porto Alegre, RS – Brazil - ZIP 91501970
☎+55 (51) 3308 6258 – Fax +55 (51) 3308 7198
http://www.iq.ufrgs/ppgq - e-mail: ppgq_iq@ufrgs.br

## 7. Bibliography

- N. Davidson, Statistical Mechanics, McGraw-Hill, 1962.
- D. A. McQuarrie, Statistical Mechanics, Harper & Row, 1976.
- A. Maczek, Statistical Thermodynamics, Oxford University Press, 1999.
- D. A. McQuarrie and J. T. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.
- M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Clarendon Press, 1987.
- D. Frenkel and B. Smith, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 1996.
- D. C. Rapaport, The Art of Molecular Dynamics Simulation, Cambridge University Press, 1997.
- A. R. Leach, Molecular Modelling: Principles and Applications, Addison-Wesley, 1997.
- K. Binder and D. W. Heermann, Monte Carlo Simulation in Statistical Physics: An Introduction, 3ª Ed., Springer Verlag, 1998.
- H. J. C. Berendsen, Simulating the Physical World, Cambridge, 2007.
- N. H. Morgon and K. Coutinho, Métodos de Química Teórica e Modelagem Molecular , Ed. Livraria da Física, 2008.
- Scientific papers.