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

1. Identification

Code and title: QUP 142 – Advanced Statistical Thermodynamics
Professor: Hubert Stassen
Level: Master and Doctorate
Credit hours: 3
Revised: June_2020

2. Summary

Statistical Mechanics of Real Systems, Fluctuations, Temporal Dependence

3. Objective

Introduce the Physical-Chemical Concepts of Real Systems and their Temporal Dependence at the Microscopic Level

4. Contents

- Classical Mechanics: Initial Conditions, Equations of Motion, Liouville Equation, Phase Space
- Review of Thermodynamics-Statistics of Ideal Systems: Microcanonical and Canonical Ensembles, Thermodynamic Functions, Gases, Crystals
- Liquids and Solutions: Distribution Functions
- Dynamic Means: Temporal Correlation Function, Thermal Fluctuations
- Wiener-Khintchine Theorem: Spectral Density, Fourier Transform
- Dynamic Variables: Density, Current, Van Hove Correlation Function, Wave Vector, Reciprocal Space, Dynamic Structure Factor
- Diffraction: Experimental Principles
- Spectroscopy: Bandwidth, Spectral Moments
- Transport Phenomena: Self-Diffusion Example, Green-Kubo Relationships
- Langevin's Equation: Float-Dissipation Theorem, Brownian Motion
- Linear Response Theory: Susceptibility, Dielectric Relaxation

5. Assessment

List of exercises, presentation and discussion of scientific articles. 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

1. H. Goldstein, Classical Mechanics, 2. Ed., Addison-Wesley, 1980.
2. D.A. McQuarrie and J.T Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.
3. D.A. McQuarrie, Statistical Mechanics, Harper & Row, 1976.
4. C.G. Gray and K.E. Gubbins, Theory of Molecular Fluids, Vol. 1: Fundamentals, Clarendon Press, 1984.
5. U. Balucani and M. Zoppi, Dynamics of the Liquid State, Oxford University Press, 1994.
6. N.H. March and M.P. Tosi, Atomic Dynamics of Liquids, Macmillan Press, 1976.
7. P.A. Egelstaff, An Introduction to the Liquid State, 2. Ed., Clarendon Press, 1994.
8. R.G. Gordon, Adv. Magn. Resonance 3 (1968), 1 and references cited therein.